

COLLECTIVE MODE OF PHONON SYSTEMS
application to a linear chain

MODE COLLECTIF DE SYSTÈMES DE PHONONS
application à une chaîne linéaire

THÈSE

PRÉSENTÉE A LA FACULTÉ DES SCIENCES
DE L'UNIVERSITÉ DE GENÈVE
POUR OBTENIR LE GRADE DE DOCTEUR ÈS SCIENCES PHYSIQUES

PAR

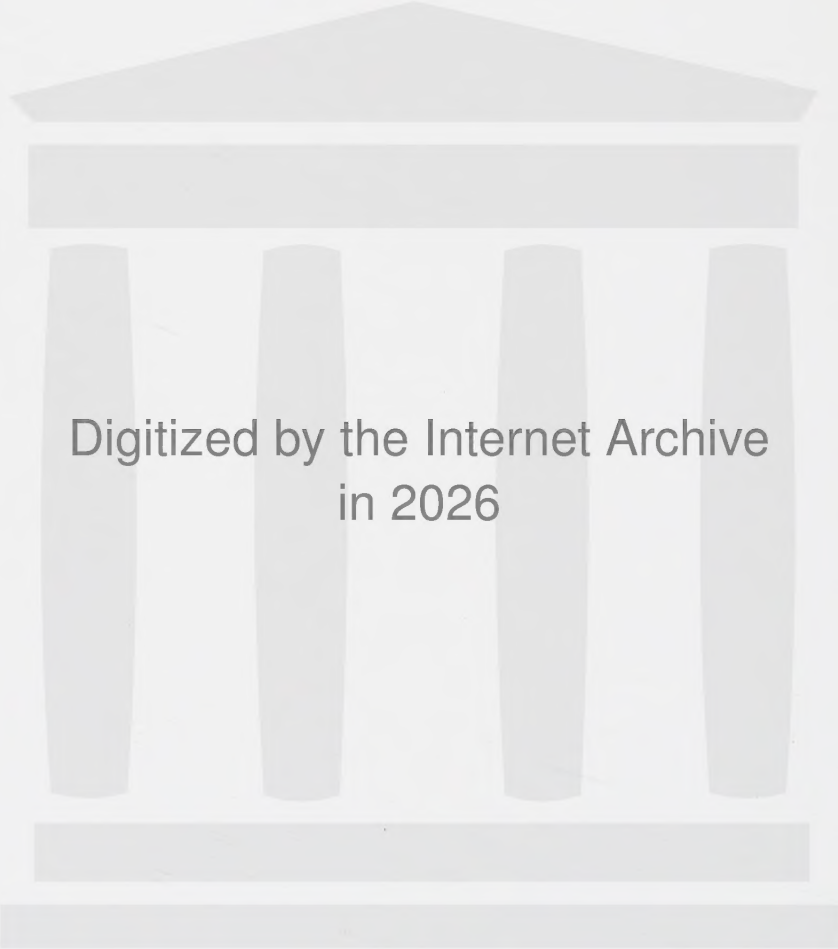
Jean-Paul Joseph MULLER

DE

SCHMERIKON (SG)

THÈSE N° 1497

1969



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UNIVERSITÉ DE GENÈVE
INSTITUT DE PHYSIQUE THÉORIQUE

FACULTÉ DES SCIENCES
PROFESSEUR CHARLES P. ENZ

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BOLOGNA
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GENÈVE, le 2 juillet 1969

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Thèse N° 1497



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RESUME

I. Par une transformation canonique, l'hamiltonien d'un cristal diélectrique est mis sous une forme où les termes anharmoniques en plus bas ordre sont les interactions à 4 phonons. L'équation de mouvement pour un mode collectif phononique de grande longueur d'onde dans une chaîne linéaire monoatomique est résolue en RPA avec conservation du nombre de phonons. Il en résulte un mode de type sonique que l'on peut décrire par un opérateur ressemblant à la densité d'énergie. Le rapport des vitesses v_{II} du son collectif et v_{I} du son ordinaire est établi explicitement pour des températures $T \ll T_{\text{D}}$ et $T \lesssim T_{\text{D}}$.

II. L'effet des interactions qui ne conservent pas le nombre de phonons sur le mode collectif dérivé dans la première partie (I) pour une chaîne linéaire monoatomique est calculé en RPA pour des températures $T \ll T_{\text{D}}$ et pour un faible couplage anharmonique $\lambda\omega_0 \ll 1$. On aboutit à une renormalisation de l'énergie collective $\Omega_q \simeq v_{\text{II}}|q|$ par un déplacement de raie qui est d'un ordre de grandeur plus petit, en puissances de $\lambda\omega_0$, que la différence entre Ω_q et la fréquence des phonons $\tilde{\omega}_q$ corrigée par des effets anharmoniques. En outre, la largeur de raie n'est plus nulle mais de l'ordre $|q|^2(\lambda\omega_0(T/T_{\text{D}}))^3$.

ABSTRACT

I. Through a canonical transformation the Hamiltonian of a dielectric crystal is brought into a form where the lowest-order anharmonic terms are 4-phonon interactions. The equation of motion for a long-wavelength collective mode of phonons in a monatomic linear chain is solved in RPA with phonon number conservation. The result is a soundlike mode described by an operator similar to the energy density. The ratio of the collective velocity v_{II} and the sound velocity v_{I} is evaluated explicitly for temperatures $T \ll T_{\text{D}}$ and $T \lesssim T_{\text{D}}$.

II. The effect of phonon-number-nonconserving interactions on the collective mode derived in Part I for a monatomic linear chain is calculated in RPA for temperatures $T \ll T_{\text{D}}$ and for weak anharmonic coupling $\lambda\omega_0 \ll 1$. It gives rise to a renormalization of the collective energy $\Omega_q \simeq v_{\text{II}}|q|$. This is shifted by an amount which is one order small in $\lambda\omega_0$ than the difference between Ω_q and the phonon frequency $\tilde{\omega}_q$ as corrected by anharmonic effects. In addition, the line width of the collective mode is no longer zero but of order $|q|^2(\lambda\omega_0(T/T_{\text{D}}))^3$.

PART I.

Introduction.

In connection with discussions of second sound the existence of a purely dynamical collective mode in a phonon system, in addition to the usual transport equation result, has been conjectured ^(1,2).

In analogy with collective excitations of many-body systems (plasmon, zero sound), ENZ ⁽¹⁾ proposed the equation of motion method of SAWADA *et al.* ⁽³⁾. For this method to be applicable, the crystal Hamiltonian (see (1.1)) has to be reducible to a form analogous to the Hamiltonian of a many-body system with central two-body interactions:

$$H = \sum_k \epsilon_k a_k^* a_k + \sum_{pqk} \frac{v_k}{2} a_{p+k}^* a_{q-k}^* a_q a_p$$

that means a form where:

- i) cubic anharmonic terms are missing;
- ii) quartic anharmonic terms conserve the number of phonons;
- iii) the coefficient $C_{k_1, k_2, k_3, k_4}^{(4)}$ has to factorize in a way which will be specified later;
- iv) higher than quartic anharmonic terms are negligible.

Whereas the last condition leads to good approximations in phonon problems, it is not easy to satisfy the three previous ones. In addition, we consider only temperatures such that the zero-point energy is irrelevant.

⁽¹⁾ C. P. ENZ: *Bull. Am. Phys. Soc.*, **9**, 278 (1964).

⁽²⁾ C. P. ENZ: in *Mathematical Methods in Solid State and Superfluid Theory, Scottish Universities' Summer School, St. Andrews, 1967*, edited by R. C. CLARK and G. H. DERRICK (Edinburgh, 1969), p. 339.

⁽³⁾ K. SAWADA, K. A. BRÜCKNER, N. FUKUDA and R. BROUT: *Phys. Rev.*, **108**, 507 (1957).

As was remarked in ref. (1) and (2) a linear chain model with only fourth-order anharmonic terms which conserve the number of phonons satisfies exactly condition iii).

The aim of the present work is to show that the problem can be solved similarly by considering cubic as well as quartic anharmonic terms. This is achieved with the aid of a unitary transformation of the Hamiltonian. Condition iii) is then true for a linear chain in the limit of small momentum.

While in 3-dimensional systems the unitary transformation of the Hamiltonian (see Sect. 1) still allows us to eliminate the cubic anharmonic terms to lowest order, the factorization property iii) cannot be maintained exactly, even in the limit of small momentum. For this reason, we restrict ourselves to the linear chain model, although we are aware of the problem of its dynamic stability (4).

1. - Canonical transformation.

The crystal Hamiltonian is (5,6),

$$(1.1) \quad H = E_0 + H_0 + \sum_{n \geq 3} H_n,$$

where

$$(1.1') \quad H_0 = \sum_k \omega_k b_k^* b_k$$

is the harmonic part, E_0 the zero-point energy, b_k^* creates a phonon with momentum $\mathbf{k}$ and polarization j ($j = 1, 2, 3$) in the branch μ ($\mu = 1, 2, \dots, B$; B = number of basis atoms) and $\pm k \equiv (\pm \mathbf{k}, \mu, j)$.

$$(1.2) \quad [b_k, b_{k'}^*]_- = \delta_{k,k'},$$

$$(1.1'') \quad H_n = \frac{1}{n!} \sum_{k_1, \dots, k_n} C_{k_1, \dots, k_n}^{(n)} Q_{k_1} \dots Q_{k_n}$$

is the n -th anharmonic term and

$$(1.3) \quad Q_k = Q_{-k}^* = \frac{1}{\sqrt{2}} (b_k + b_{-k}^*).$$

(4) N. D. MERMIN: *Phys. Rev.*, **176**, 250 (1968).

(5) G. LEIBFRIED and W. LUDWIG: in *Solid State Physics*, vol. **12**, edited by F. SEITZ and D. TURNBULL (New York and London, 1961), p. 275.

(6) C. P. ENZ: *Ann. of Phys.*, **46**, 114 (1968).

As discussed, *e.g.*, by ISHIKAWA ⁽⁷⁾, the n -th anharmonic term H_n is of order $(u/r_0)^{n-2}$ where u is an average atomic displacement and r_0 the nearest neighbour spacing. For low temperatures $T \ll T_D$ (T_D = Debye temperature) $|u/r_0| \ll 1$.

Let us perform a unitary transformation according the general scheme of ⁽⁸⁾ and ⁽⁹⁾

$$(1.4) \quad \tilde{H} = \exp [iS] H \exp [-iS] = \\ = E_0 + H_0 + (H_3 - i[H_0, S]) + H_4 - i[H_3, S] - \frac{1}{2} [[H_0, S], S] + \dots$$

by requiring that

$$(1.4') \quad H_3 - i[H_0, S] = 0,$$

or, in interaction representation defined by

$$A[t] \equiv \exp [iH_0 t] A \exp [-iH_0 t], \quad \dot{S}[t] = H_3[t].$$

Then the solution is, using a switch-on condition,

$$(1.4'') \quad S = \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^0 dt \exp [\varepsilon t] H_3[t].$$

By substitution of (1.4') into (1.4) one finds

$$(1.5) \quad \tilde{H} = E_0 + H_0 + H_4 - \frac{i}{2} [H_3, S] + O \left\{ \left| \frac{u}{r_0} \right|^3 \right\}.$$

From (1.4'') the explicit form of S in terms of phonon creation and annihilation operators is found to be

$$(1.6) \quad S = \frac{-i\sqrt{2}}{4!} \sum_{k_1 k_2 k_3} C_{k_1 k_2 k_3}^{(3)} \left\{ \frac{b_{-k_1}^* b_{-k_2}^* b_{-k_3}^*}{\omega_{k_1} + \omega_{k_2} + \omega_{k_3} - i\varepsilon} + 3 \frac{b_{-k_1}^* b_{k_2} b_{k_3}}{\omega_{k_1} - \omega_{k_2} - \omega_{k_3} - i\varepsilon} \right\} + \\ + \text{h.c.},$$

where

$$C_{k_1 k_2 k_3}^{(3)*} = C_{-k_1, -k_2, -k_3}^{(3)} \quad \text{and} \quad C_{k, -k, k'}^{(3)} = 0$$

are used.

⁽⁷⁾ K. ISHIKAWA: *Phys. Stat. Sol.*, **21**, 137 (1967).

⁽⁸⁾ S. TANI: *Progr. Theor. Phys.*, **11**, 190 (1954).

⁽⁹⁾ E. P. GROSS: in *Mathematical Methods in Solid State and Superfluid Theory, Scottish Universities' Summer School, St. Andrews, 1967*, edited by R. C. CLARK and G. H. DERRICK (Edinburgh, 1969), p. 46.

The difference between (1.6) and the transformation of ref. (7) is that the latter is defined with the principal part of the energy denominators and, consequently, does not eliminate those terms of H_3 , for which

$$\omega_{k_1} - \omega_{k_2} - \omega_{k_3} = 0.$$

By use of (1.2) and (1.3), $\tilde{H}$ takes the form

$$(1.7) \quad \begin{aligned} \tilde{H} = \tilde{E}_0 + \sum_k \omega_k b_k^* b_k + \frac{1}{4!} \sum_{k_1, \dots, k_4} \tau_{(k_1, k_2)(k_3, k_4)} b_{-k_1}^* b_{-k_2}^* b_{k_3} b_{k_4} + \\ + \frac{1}{4!} \sum_{k_1, \dots, k_4} \{(\mu_{(k_1, \dots, k_4)} b_{k_1} b_{k_2} b_{k_3} b_{k_4} + \text{h.c.}) + (\gamma_{k_1(k_2, k_3, k_4)} b_{-k_1}^* b_{k_2} b_{k_3} b_{k_4} + \text{h.c.})\} + \\ + \sum_k \{\lambda_k (b_k b_{-k} + b_k^* b_k) + \text{h.c.}\} + O\left\{\left|\frac{u}{r_0}\right|^3\right\}, \end{aligned}$$

where the coefficients are given in Appendix A in terms of $C_{k_1, k_2, k_3}^{(3)}$ and $C_{k_1, k_2, k_3, k_4}^{(4)}$. They are completely symmetric with respect to permutations of arguments k_i in the same parenthesis and proportional to

$$(1.8) \quad \Delta\left(\sum_{i=1}^4 k_i\right) = \begin{cases} 1 & \text{if } \sum_{i=1}^4 k_i = \mathbf{K} \text{ (reciprocal lattice vector),} \\ 0 & \text{otherwise.} \end{cases}$$

As in field theory, dynamical quantities will be expressed in terms of normal products. For the energy $:\tilde{H}:$, this is equivalent to setting $\tilde{E}_0 = 0$ and $\lambda_k = 0$.

2. - Equation of motion of phonon density operator in RPA.

The approximation of phonon-number conservation consists in neglecting those anharmonic terms of $:\tilde{H}:$ which create more phonons than they annihilate or vice versa. Their effect will be treated in a subsequent publication (Part II) and turns out to be a renormalization of the collective mode energy $\Omega_q \simeq v_{\text{II}}|q|$. This renormalization is one order of magnitude smaller, in terms of $\beta v_{\text{I}} \cdot |q| \ll 1$, than $|v_{\text{II}} - v_{\text{I}}| \cdot |q|$, where v_{I} is the sound velocity and $\beta = (k_B T)^{-1}$. The approximate Hamiltonian

$$(2.1) \quad \bar{H} = \sum_k \omega_k b_k^* b_k + \frac{1}{4!} \sum_{k_1, \dots, k_4} \tau_{(k_1, k_2)(k_3, k_4)} b_{-k_1}^* b_{-k_2}^* b_{k_3} b_{k_4}$$

has the form of a many-body Hamiltonian with 2-body forces. Therefore, the method used by SAWADA *et al.* ⁽³⁾ for the plasma oscillation of an electron gas may be used here, under the condition, however, that the coefficient $\tau_{(k_1, k_2)(k_3, k_4)}$ factorizes.

In analogy to the equation of motion of the electron density operator used in ref. ⁽³⁾ we study the equation of motion

$$(2.2) \quad \frac{1}{i} \dot{n}_k(q) = [\bar{H}, n_k(q)]_- ,$$

where

$$(2.2') \quad n_k(q) \equiv b_k^* b_{k-q} ;$$

with (2.1) we obtain:

$$\begin{aligned} \frac{1}{i} \dot{n}_k(q) = & (\omega_k - \omega_{k-q}) n_k(q) + \\ & + \frac{2}{4!} \sum_{k_1 k_2 k_3} (\tau_{(k_1, k_2)(k_3, k)} b_{-k_1}^* b_{-k_2}^* b_{k_3} b_{k-q} - \tau_{(q-k, k_1)(k_2, k_3)} b_k^* b_{-k_1}^* b_{k_2} b_{k_3}) . \end{aligned}$$

RPA consists in approximating the 4-phonon term by

$$(2.3) \quad b_{k_1}^* b_{k_2}^* b_{k_3} b_{k_4} \simeq b_{k_1}^* \underbrace{b_{k_2}^* b_{k_3}} b_{k_4} + b_{k_1}^* \underbrace{b_{k_2}^* b_{k_4}} b_{k_3} + \underbrace{b_{k_1}^* b_{k_3}^*} b_{k_2} b_{k_4} + \underbrace{b_{k_1}^* b_{k_2}^*} b_{k_3} b_{k_4} ,$$

where

$$(2.3') \quad \dots \underbrace{b_k^* \dots b_{k'}} \dots \equiv \delta_{k, k'} n_k \dots ,$$

$$(2.4) \quad n_k \equiv \langle n_k(0) \rangle ,$$

and the average is defined by

$$(2.4') \quad \langle A \rangle = \text{Tr} (\exp [-\beta \bar{H}] A) / \text{Tr} (\exp [-\beta \bar{H}]) .$$

In this approximation

$$\begin{aligned} (2.5) \quad \frac{1}{i} \dot{n}_k(q) \simeq & (\omega_k - \omega_{k-q}) n_k(q) + \\ & + \frac{1}{3!} \sum_{k' k''} n_{k'} (\tau_{(k'', -k') (k', k)} b_{-k''}^* b_{k-q} - \tau_{(k'', -k') (k', k-q)} b_k^* b_{-k''}) + \\ & + \frac{1}{3!} (n_{k-q} - n_k) \sum_{k' k''} \tau_{(-k', q-k) (k'', k)} b_{k'}^* b_{k''} , \end{aligned}$$

where

$$k = (\mathbf{k}, \mu, j); \quad k' = (\mathbf{k}', \mu', j'); \quad k - q = (\mathbf{k} - \mathbf{q}, \mu, j).$$

The sums on the right-hand side become very simple in the case of a monatomic linear chain, for which no branch and polarization indices (μ, j) are needed, and where the wave vector is simply

$$(2.6) \quad k = \frac{m}{N} \cdot \frac{2\pi}{a}, \quad -\frac{N}{2} < m = \text{integer} \leq +\frac{N}{2},$$

where a is the lattice constant and Na the length of the periodic chain. (See Appendix B for the dynamics of a monatomic linear chain with nearest-neighbour interactions.) Then

$$(2.7) \quad \frac{1}{i} \dot{n}_k(q) \simeq n_k(q)(\omega_k - \omega_{k-q}) + \frac{1}{3!} (n_{k-q} - n_k) \sum_{K, k'} \tau_{(q-k, -k')(\mathbf{k}, \mathbf{K}+\mathbf{k}'-q)} n_{k'}(q-K) + \\ + \sum_K \left(n_{k-K}(q-K) \frac{1}{3!} \sum_{k'} n_{k'} \tau_{(K-k, -k')(\mathbf{k}', \mathbf{k})} - n_k(q+K) \frac{1}{3!} \sum_{k'} n_{k'} \tau_{(K-k+q, -k')(\mathbf{k}', \mathbf{k}-q)} \right).$$

We are interested in a long-wavelength excitation, *i.e.* in the limit $|q| \ll \pi/a$. In this limit Umklapp processes $K \neq 0$ may be neglected since they are one order in $|q|$ smaller than the normal processes. This is because the fraction of the first Brillouin zone, which satisfies the Umklapp condition is of order $|q|$. Then, for the monatomic linear chain considered here (see Appendix C)

$$(2.8) \quad \tau_{(q-k, -k')(\mathbf{k}, \mathbf{k}'-q)}|_{|q| \ll \pi/a} \simeq 3! \frac{\lambda}{N} \sqrt{\omega_k \omega_{k-q} \omega_{k'} \omega_{k'-q}},$$

which is completely factorized.

3. - Renormalization of phonon frequency.

We define a renormalized frequency $\bar{\omega}_k$ by the equation of motion in RPA,

$$(3.1) \quad \frac{1}{i} \dot{b}_k^*(t) \simeq \bar{\omega}_k b_k^*(t)$$

and calculate

$$\frac{1}{i} \dot{b}_k^*(t) = [\bar{H}, b_k^*(t)]_- = \omega_k b_k^*(t) + \frac{2}{4!} \sum_{k_1 k_2 k_3} \tau_{(k_1, k_2)(k_3, k)} b_{-k_1}^* b_{-k_2}^* b_{k_3}.$$

and making use of

$$(3.7) \quad \beta^{-1} \sum_{\sigma} \tilde{g}(k, i\sigma) = n_k$$

the renormalization (3.2) is readily seen to be given by the self-energy term

$$(3.8) \quad \text{Diagram 1} \cong \beta^{-1} \sum_{\ell, \sigma} \text{Diagram 2} .$$

Substituting (3.4) and (3.8) into (3.5) and making use of (3.2) leads to

$$(3.9) \quad \tilde{g}(k, i\sigma) \simeq (\bar{\omega}_k + i\sigma)^{-1} ,$$

from which, according (3.7), the mean phonon number follows self-consistently as

$$(3.10) \quad n_k \simeq \bar{n}_k \equiv ([\exp \beta \bar{\omega}_k] - 1)^{-1} .$$

Substitution of (2.8) and (3.10) into (3.2) allows to write

$$(3.11) \quad \bar{\omega}_k = \gamma(\lambda, \beta) \cdot \omega_k ,$$

where

$$(3.12) \quad \gamma^2(\lambda, \beta) = \gamma(\lambda, \beta) + \Theta \cdot J(\beta \bar{\omega}_0) ,$$

$$(3.12') \quad \Theta \equiv \lambda \cdot \beta^{-1} ,$$

and, with $\bar{\omega}_0 = \bar{\omega}_{k_{\max}}$,

$$(3.13) \quad J(\beta \bar{\omega}_0) \equiv \beta \cdot \frac{1}{N} \sum_k \bar{\omega}_k \bar{n}_k .$$

4. - Collective-mode operator and eigenvalue equation.

The simplest collective-mode operator is bilinear in the phonon creation and annihilation operators. Thus, the operator which creates a collective mode with momentum q is of the form ⁽³⁾

$$(4.1) \quad c_q^* = \sum_k \alpha_{k, k-q}^* n_k(q) ,$$

where $n_k(q)$ is given by (2.2'). To a certain approximation to be specified this c_q^* has to satisfy the analogue of the relations (1.2) and (3.1)

$$(4.2) \quad \langle [c_q, c_q^*]_- \rangle_0 = \delta_{a, a'} ,$$

$$(4.3) \quad \frac{1}{i} \dot{c}_q^* = \Omega_q c_q^* ,$$

where

$$\langle A \rangle_0 \equiv \text{Tr} (\exp [-\beta \bar{H}_0] A) / \text{Tr} (\exp [-\beta \bar{H}_0]) ,$$

$$\bar{H}_0 \equiv \sum_k \bar{\omega}_k b_k^* b_k .$$

These two conditions determine the coefficients $\alpha_{k, k-q}^*$ and the collective energy Ω_q .

By substitution of (4.1), (2.7) with $K = 0$, (2.8) and (3.2) into (4.3), one has

$$\sum_k \alpha_{k, k-q}^* (\Omega_q - (\bar{\omega}_k - \bar{\omega}_{k-q})) n_k(q) = N_q^* \sum_{k'} \sqrt{\omega_{k'} \omega_{k'-q}} n_{k'}(q) ,$$

where

$$(4.4) \quad N_q^* \equiv \lambda \cdot \frac{1}{N} \sum_k \alpha_{k, k-q}^* \sqrt{\omega_k \omega_{k-q}} (\bar{n}_{k-q} - \bar{n}_k) .$$

The linear independence of the operators $n_k(q)$ with respect to k implies

$$(4.5) \quad \alpha_{k, k-q}^* (\Omega_q - (\bar{\omega}_k - \bar{\omega}_{k-q})) = N_q^* \sqrt{\omega_k \omega_{k-q}} .$$

Substitution into (4.4) yields the eigenvalue equation:

$$(4.6) \quad F_q(\Omega_q) = 1 ,$$

where « the dynamical function »

$$(4.6') \quad F_q(z) \equiv \lambda \cdot \frac{1}{N} \sum_k \frac{\omega_k \omega_{k-q}}{z - (\bar{\omega}_k - \bar{\omega}_{k-q})} (\bar{n}_{k-q} - \bar{n}_k)$$

plays the same role as the dynamical matrix of a harmonic crystal.

The normalization factor N_q^* follows with (4.6') from

$$\langle [c_q, c_q^*]_- \rangle_0 = N \cdot |N_q|^2 \cdot \delta_{a, a'} \cdot \frac{1}{N} \sum_k \frac{\omega_k \omega_{k-q} (\bar{n}_{k-q} - \bar{n}_k)}{(\Omega_q - (\bar{\omega}_k - \bar{\omega}_{k-q}))^2} = -\frac{N}{\lambda} \cdot |N_q|^2 \cdot \left(\frac{dF_q(z)}{dz} \right)_{z=\Omega_q} \delta_{a, a'} ,$$

which, together with (4.2) gives

$$(4.7) \quad |N_q|^2 = -\frac{\lambda}{N} \left(\frac{dF_q(z)}{dz} \right)_{z=\Omega_q}^{-1} .$$

5. - Discussion of the eigenvalue equation.

The singularities of the function $F_q(z)$ lie on the interval

$$\min |\bar{\omega}_k - \bar{\omega}_{k-q}| = 0 \leq |z| \leq \bar{\omega}_q = \max |\bar{\omega}_k - \bar{\omega}_{k-q}|.$$

Since $\bar{\omega}_k = \bar{\omega}_{-k}$ and consequently $\bar{n}_k = \bar{n}_{-k}$, a change $k \rightarrow q-k$ in the summation allows us to write $F_q(z)$ in the form

$$(5.1) \quad F_q(z) = \lambda \cdot \frac{1}{N} \sum_k \omega_k \omega_{k-q} \frac{(\bar{\omega}_k - \bar{\omega}_{k-q})(\bar{n}_k - \bar{n}_{k-q})}{(\bar{\omega}_k - \bar{\omega}_{k-q})^2 - z^2},$$

which is reported as function of z^2 in Fig. 1.

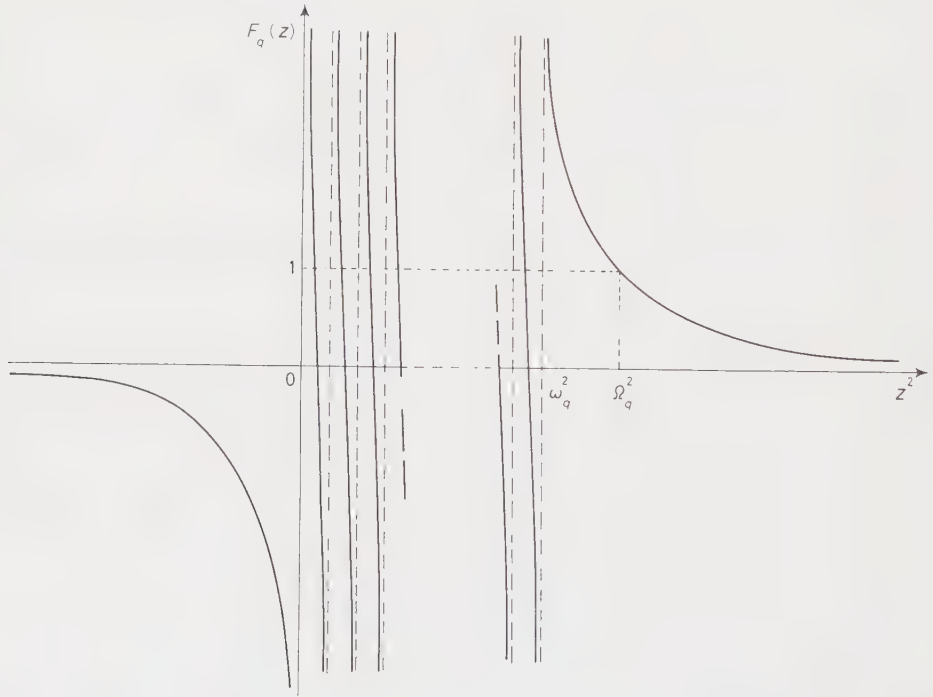


Fig. 1. - The « dynamical function » $F_q(z)$ vs. real z^2 for $\lambda > 0$. $F_q(\Omega_q) = 1$ gives the energy $\Omega_q \simeq v_{\text{H}} \cdot |q|$ of the collective mode.

Therefore, $F_{-q}(z) = F_q(z)$ and $\Omega_{-q} = \Omega_q$, i.e. if Ω_q is a solution, then Ω_{-q} also is.

It follows that for $\lambda > 0$, there exists a real solution $\Omega_q^2 > \bar{\omega}_q^2 > 0$ (see Fig. 1) and because of an arbitrariness of sign in eq. (4.3) we may restrict our-

selves to

$$(5.2) \quad \Omega_q > \bar{\omega}_q > 0.$$

For $\lambda < 0$ the solution of (4.6) is $\Omega_q^2 < 0$, which is unphysical.

In the long-wavelength limit $|q| \ll \pi/a$ the solution is soundlike,

$$\Omega_q \simeq v_{\text{II}} \cdot |q| + O\{|q|^2\}$$

and (5.1) evaluated to lowest order in q gives

$$(5.3) \quad F_q(v_{\text{II}}|q|) \simeq \lambda \frac{1}{N} \sum_k \frac{\omega_k^2 (\text{d}\bar{\omega}_k/\text{d}k)^2 (\text{d}\bar{n}_k/\text{d}\bar{\omega}_k)}{(\text{d}\bar{\omega}_k/\text{d}k)^2 - v_{\text{II}}^2},$$

which may be evaluated explicitly in the limit $N \rightarrow \infty$ where

$$(5.4) \quad \frac{1}{N} \sum_k \rightarrow \frac{a}{2\pi} \int_{-\pi/a}^{+\pi/a} \text{d}k.$$

From Appendix B, eq. (B.1), we have

$$\omega_k = \omega_0 \cdot \left| \sin \frac{ak}{2} \right|$$

and with the maximum renormalized frequency from (3.11) we obtain

$$(5.5) \quad \begin{cases} \bar{\omega}_k = \bar{\omega}_0 \left| \sin \frac{ak}{2} \right|, & \frac{\text{d}\bar{\omega}_k}{\text{d}k} = v_{\text{I}} \text{sign}(k) \cdot \cos \frac{ak}{2}, \\ \bar{\omega}_0 = \gamma(\lambda, \beta) \omega_0, & v_{\text{I}} \equiv \frac{a\bar{\omega}_0}{2}. \end{cases}$$

Substitution of (3.10) and (5.5) into (5.3) gives, making use of (5.4) and the dimensionless variable (3.12')

$$(5.6) \quad F_q(v_{\text{II}}|q|) \simeq \frac{\Theta(\beta\bar{\omega}_0)^2}{\pi\gamma^2} \int_{-\pi/2}^{+\pi/2} \text{d}x \frac{\cos^2 x \cdot \sin^2 x \cdot \exp[\beta\bar{\omega}_0 \cdot \sin x]}{((v_{\text{II}}/v_{\text{I}})^2 - \cos^2 x)(\exp[\beta\bar{\omega}_0 \cdot \sin x] - 1)^2},$$

or with $y \equiv \beta\bar{\omega}_0 \cdot \sin x$

$$(5.7) \quad F_q(v_{\text{II}}|q|) \simeq \frac{2\Theta}{\pi\gamma^2} \cdot \frac{1}{\beta\bar{\omega}_0} \int_0^{\beta\bar{\omega}_0} \text{d}y \frac{\sqrt{1 - (y/\beta\bar{\omega}_0)^2} \cdot y^2 \cdot \exp[y]}{((v_{\text{II}}/v_{\text{I}})^2 - 1 + (y/\beta\bar{\omega}_0)^2)(\exp[y] - 1)^2}.$$

The different approximations of this integral are determined by the behaviour of the function

$$\frac{y^2 \cdot \exp[y]}{(\exp[y] - 1)^2}.$$

The following limits are expected to give accurate results:

a) $\beta\bar{\omega}_0 \sim 1$, i.e. $T \sim \gamma(\lambda, T) \cdot T_D$ high temperatures,

b) $\beta\bar{\omega}_0 \geq 10$, i.e. $T \lesssim 10^{-1} \gamma(\lambda, T) \cdot T_D$ low temperatures,

where the Debye temperature at absolute zero is defined by

$$(5.8) \quad \omega_0 = k_B T_D.$$

$\gamma(\lambda, T)$ will turn out to be of order $\frac{3}{2}$ for a) and 1 for b).

The approximations to be used in (5.7) consist in setting

$$(5.9) \quad \begin{cases} a) & y^2 \exp[y] (\exp[y] - 1)^{-2} \simeq 1 \text{ if } \beta\bar{\omega}_0 \sim 1, \\ b) & \sqrt{1 - \left(\frac{y}{\beta\bar{\omega}_0}\right)^2} \simeq 1, \quad \text{if } \beta\bar{\omega}_0 \geq 10. \end{cases}$$

6. - High-temperature solution.

This solution is of interest below but close to the Debye temperature.

By use of the form (5.6) in the approximation (5.9a) we have, introducing the dimensionless eigenvalue

$$(6.1) \quad \alpha \equiv (v_{\text{II}}/v_{\text{I}})^2 - 1,$$

$$(6.2) \quad F_a(v_{\text{II}}|q|) \simeq \frac{\Theta}{\pi\gamma^2} \{(\alpha + 1) \cdot \varphi(\alpha) - \pi\},$$

where

$$(6.2') \quad \varphi(\alpha) \equiv \int_{-\pi/2}^{+\pi/2} \frac{dx}{\alpha + 1 - \cos^2 x}.$$

With the substitution

$$z = \exp[2ix],$$

$$4 \cos^2 x = z + 2 + \frac{1}{z},$$

integration in the complex z -plane yields

$$(6.2'') \quad \varphi(\alpha) = 2i \oint_{|z|=1} \frac{dz}{z^2 - 2(2\alpha + 1)z + 1} = \frac{\pi}{+\sqrt{\alpha(\alpha + 1)}}.$$

With (6.2) and (6.2'') the eigenvalue equation (4.6) reduces to

$$(6.3) \quad 1 \simeq \frac{\Theta}{\gamma^2} \left(\sqrt{\frac{\alpha + 1}{\alpha}} - 1 \right)$$

and the eigenvalue is

$$(6.3') \quad \alpha = \frac{\Theta^2}{\gamma^2(\gamma^2 + 2\Theta)}.$$

By use of (5.4) and (5.5) the parameter $J(\beta\bar{\omega}_0)$ defined in (3.13) becomes

$$(6.4) \quad J(\beta\bar{\omega}_0) = \frac{2}{\pi} \int_0^{\pi/2} dx \frac{\beta\bar{\omega}_0 \cdot \sin x}{\exp[\beta\bar{\omega}_0 \cdot \sin x] - 1}.$$

Using the expansion which generates the Bernoulli numbers B_n

$$(6.5) \quad \frac{y}{\exp[y] - 1} = \sum_{n=0}^{\infty} B_n \frac{y^n}{n!},$$

$|y| < 2\pi,$

we have

$$(6.6) \quad J(y) =$$

$$= B_1 \cdot \frac{2}{\pi} \cdot y + \sum_{n=0}^{\infty} B_{2n} \frac{y^{2n}}{(2^n \cdot n!)^2}.$$

From (3.12) and the requirement

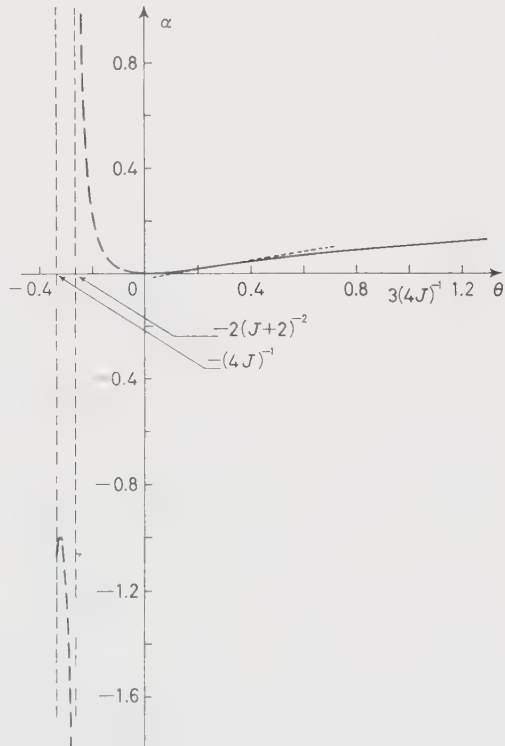


Fig. 2. - The eigenvalue $\alpha(J, \Theta) \equiv (v_{II}/v_I)^2 - 1$ (equations (6.3') and (6.7)) vs. $\Theta \equiv \lambda \cdot \beta^{-1} = \lambda k_B T$ for temperatures $T \lesssim T_D$ and $J = \frac{3}{4}$. --- is the « - » sheet of $\sqrt{(\alpha + 1)/\alpha}$, — is the « + » sheet of $\sqrt{(\alpha + 1)/\alpha}$.

$\gamma \geq 0$ it follows that

$$(6.7) \quad \gamma = \frac{1}{2} (1 + \sqrt{1 + 4J \cdot \Theta}) .$$

From (6.4) we obtain

$$(6.8) \quad \frac{y}{\exp[y] - 1} < J(y) < 1, \quad \frac{dJ(y)}{dy} < 0 .$$

Figure 2 shows the behaviour of $\alpha(J, \Theta)$, eq. (6.3'), for fixed J . The value chosen, $J = \frac{3}{4}$, corresponds to $\beta\bar{\omega}_0 \leq 1$, ($J(1) \simeq 0.724$). From the condition $\alpha \geq 0$ and the limitation to the « + » sheet of $\sqrt{\alpha + 1/\alpha}$ it follows, that only the region $\Theta \geq 0$ is physical, in agreement with the discussion of Fig. 1.

For $\Theta < -1/4J$, γ is imaginary, which has to be excluded.

7. - Low-temperature solution.

The approximation (5.9b) applied to (5.7) gives

$$(7.1) \quad F_q(v_{\text{II}}|q) \simeq \frac{2\Theta}{\pi\gamma^2} \cdot \frac{1}{\beta\bar{\omega}_0} \int_0^{\beta\bar{\omega}_0} \frac{dy \cdot y^2 \cdot \exp[y]}{(\alpha + (y/\beta\bar{\omega}_0)^2)(\exp[y] - 1)^2} .$$

At very low temperatures ($\beta\bar{\omega}_0 \rightarrow \infty$) one would think that the term $(y/\beta\bar{\omega}_0)^2$ in the dominator can also be neglected, because the resulting error is multiplied by the factor $y^2 \exp[y]/(e^y - 1)^2$ which tends very rapidly to zero in the region $1 < y \leq \beta\bar{\omega}_0$ where $y/\beta\bar{\omega}_0$ becomes comparable to or larger than α . Although we shall see below that this is not so, we quote the result obtained in this way for comparison with ref. (2):

$$F_q(v_{\text{II}}|q) \simeq \frac{2\Theta}{\pi\gamma^2} \cdot \frac{1}{\beta\bar{\omega}_0} \cdot \frac{1}{\alpha} \int_0^\infty dy \frac{y^2 \exp[y]}{(\exp[y] - 1)^2} .$$

Integration by parts leads to the integral⁽¹¹⁾

$$\int_0^\infty \frac{y dy}{\exp[y] - 1} = \frac{\pi^2}{6}$$

⁽¹¹⁾ I. S. GRADSTEYN and I. M. RYZHIK: *Tables of Integrals, Series and Products*, translation edited by A. JEFFREY (New York, 1965); form. 3.411/2.

so that the eigenvalue equation (4.6) implies

$$(7.2) \quad \alpha \simeq \frac{2\pi\Theta}{3\beta\omega_0} \cdot \frac{1}{\gamma^3},$$

or with (6.1)

$$(7.2') \quad v_{\text{II}} \simeq v_{\text{I}} \left(1 + \frac{\pi\Theta}{3\beta\omega_0} \cdot \frac{1}{\gamma^3} \right).$$

This is identical with eq. (32) of ref. (2) provided ω_0 is replaced by ω_{D} and the phonon renormalization is neglected ($\gamma = 1$). In order to get a better approximation of (7.1) we approximate the integrand by

$$\begin{aligned} & \frac{1}{\alpha} \frac{y^2 \exp[y]}{(\exp[y] - 1)^2} && \text{for small } y, \\ & (\beta\bar{\omega}_0)^2 \frac{\exp[y]}{(\exp[y] - 1)^2} && \text{for large } y, \end{aligned}$$

the optimal separation point of the integral being $y = \sqrt{\alpha}\beta\bar{\omega}_0$ for which these two functions are equal. Hence

$$(7.3) \quad F_q(v_{\text{II}}|q|) \simeq \frac{2\Theta}{\pi\gamma^2} \cdot \frac{1}{\beta\bar{\omega}_0} \left\{ \frac{1}{\alpha} \int_0^{\sqrt{\alpha}\beta\bar{\omega}_0} dy \frac{y^2 \exp[y]}{(\exp[y] - 1)^2} + (\beta\bar{\omega}_0)^2 \int_{\sqrt{\alpha}\beta\bar{\omega}_0}^{\beta\bar{\omega}_0} dy \frac{\exp[y]}{(\exp[y] - 1)^2} \right\}.$$

From (7.2) we know by substitution of $\Theta = \lambda\omega_0/\beta\omega_0$ that

$$\alpha \leq \frac{2\pi}{3} \cdot \frac{\lambda\omega_0}{\gamma} \cdot \frac{1}{(\beta\bar{\omega}_0)^2}.$$

If the coupling constant λ satisfies $\lambda\omega_0 < 3$ we have $y \leq \sqrt{\alpha}\beta\bar{\omega}_0 < 2\pi$ and (6.5) is applicable to the first integral of (7.3), which after integration by parts takes the form

$$\frac{2}{\alpha} \int_0^{\sqrt{\alpha}\beta\bar{\omega}_0} dy \frac{y}{\exp[y] - 1} - \frac{(\beta\bar{\omega}_0)^2}{\exp[\sqrt{\alpha}\beta\bar{\omega}_0] - 1}.$$

In the second integral of (7.3) which gives

$$(\beta\bar{\omega}_0)^2 \left(\frac{1}{\exp[\sqrt{\alpha}\beta\bar{\omega}_0] - 1} - \frac{1}{\exp[\beta\bar{\omega}_0] - 1} \right)$$

the term of order $\beta\bar{\omega}_0(\exp[\beta\bar{\omega}_0] - 1)$ has to be neglected for consistency with

the approximation (5.9b). Then, with $\gamma \cdot \beta \omega_0 = \beta \bar{\omega}_0$,

$$(7.4) \quad F_s(v_{\text{II}}|q|) \simeq \frac{4\lambda\omega_0}{\pi\gamma\alpha(\beta\bar{\omega}_0)^2} \cdot \int_0^{\sqrt{\alpha}\beta\bar{\omega}_0} dy \cdot \frac{y}{\exp[y]-1}.$$

The eigenvalue equation (4.6) leads to

$$(7.5) \quad \frac{\pi\gamma}{4\lambda\omega_0} \cdot \sqrt{\alpha}\beta\bar{\omega}_0 \simeq \frac{1}{\sqrt{\alpha}\beta\bar{\omega}_0} \int_0^{\sqrt{\alpha}\beta\bar{\omega}_0} \frac{dy \cdot y}{\exp[y]-1}.$$

This equation could be solved graphically for $\sqrt{\alpha}\beta\bar{\omega}_0$ with $\pi\gamma/4\lambda\omega_0$ as parameter by use of Table 27.1 of ref. (12) for the Debye function

$$\frac{1}{x} \int_0^x \frac{t dt}{\exp[t]-1};$$

we prefer an approximate algebraic solution. Substitution of (6.5) into (7.4) gives

$$F_s(v_{\text{II}}|q|) = \frac{4\lambda\omega_0}{\pi\gamma\alpha(\beta\bar{\omega}_0)^2} \sum_{n=0}^{\infty} \frac{B_n}{(n+1)!} (\sqrt{\alpha}\beta\bar{\omega}_0)^{n+1}.$$

The rapid convergence of this series allows us to write approximatively, with $\beta\bar{\omega}_0 = \gamma\beta\omega_0$,

$$(7.6) \quad F_s(v_{\text{II}}|q|) \simeq \frac{4\lambda\omega_0}{\pi\gamma^2\sqrt{\alpha}\beta\omega_0} \left\{ 1 - \frac{\gamma}{4}\sqrt{\alpha}\beta\omega_0 + \frac{\gamma^2}{36}\alpha \cdot (\beta\omega_0)^2 \right\}.$$

In the variables $u \equiv \lambda\omega_0$ and (see (5.8)) $T/T_D \equiv (\beta\omega_0)^{-1}$ the solution of (4.6) at low temperatures then is

$$(7.7) \quad \alpha \simeq \frac{81}{4} \left(\frac{1}{\gamma u} \cdot \frac{T}{T_D} \right)^2 \left[\pm \sqrt{(\pi\gamma + u)^2 - \left(\frac{4}{3}u \right)^2} - (\pi\gamma + u) \right]^2.$$

This expression is valid under the condition of the development (6.5), i.e. if

$$|\sqrt{\alpha}\gamma| \frac{T_D}{T} < 2\pi.$$

(12) *Handbook of Mathematical Functions*, edited by M. ABRAMOWITZ and I. A. STEGUN (National Bureau of Standards, 1964).

The integral $J(\beta\bar{\omega}_0)$ given by (6.4) which enters the equation for γ (3.12), evaluated in the same approximation (5.9b) is

$$(7.8) \quad J(\beta\bar{\omega}_0) = \frac{2}{\pi\beta\bar{\omega}_0} \int_0^{\beta\bar{\omega}_0} \frac{dy}{\sqrt{1 - (y/\beta\bar{\omega}_0)^2}} \cdot \frac{y}{\exp[y] - 1} =$$

$$= \frac{2}{\pi\beta\bar{\omega}_0} \int_0^{\beta\bar{\omega}_0} dy \sqrt{1 - \left(\frac{y}{\beta\bar{\omega}_0}\right)^2} \left(\frac{y}{\exp[y] - 1} + \frac{d}{dy} \frac{y^2}{\exp[y] - 1} \right) \simeq \frac{\pi}{3\beta\bar{\omega}_0} \quad (11).$$

8. - Normalization of the collective-mode operator c_a^* .

Substitution of (4.5) into the definition (4.1) leads to the operator

$$(8.1) \quad c_a^* = N_a^* \sum_k \frac{\sqrt{\omega_k \omega_{k-a}}}{\Omega_a - (\bar{\omega}_k - \bar{\omega}_{k-a})} n_k(q),$$

where $\Omega_a \simeq v_{\text{II}} \cdot |q|$, ($|q| \ll \pi/\alpha$), is the solution of the eigenvalue equation (4.6) derived in the preceding Sections.

The normalization N_a^* is given by (4.7), where $dF_q(z)/dz$ follows from eq. (5.1)

$$\left. \frac{dF_q(z)}{dz} \right|_{z=v_{\text{II}}|q|} = \frac{2\lambda v_{\text{II}}|q|}{\gamma^2} \cdot \frac{1}{N} \sum_k \bar{\omega}_k \bar{\omega}_{k-a} \frac{(\bar{\omega}_k - \bar{\omega}_{k-a})(\bar{n}_k - \bar{n}_{k-a})}{[(\bar{\omega}_k - \bar{\omega}_{k-a})^2 - v_{\text{II}}^2 |q|^2]^2}.$$

To lowest order in $|q|$, this expression becomes, by use of (5.4), (5.5), (3.10)

$$z \cdot \left. \frac{dF_q(z)}{dz} \right|_{z=v_{\text{II}}|q|} \simeq \frac{2\lambda v_{\text{II}}^2}{\gamma^2} \cdot \frac{a}{\pi} \int_0^{\pi/\alpha} dk \frac{(d\bar{\omega}_k/dk)^2 (d\bar{n}_k/d\bar{\omega}_k) \cdot \bar{\omega}_k^2}{[(d\bar{\omega}_k/dk)^2 - v_{\text{II}}^2]^2}$$

and with (3.12')

$$(8.2) \quad z \cdot \left. \frac{dF_q(z)}{dz} \right|_{z=v_{\text{II}}|q|} \simeq$$

$$\simeq -\frac{2\Theta}{\gamma^2} (\alpha + 1)(\beta\bar{\omega}_0)^2 \cdot \frac{2}{\pi} \int_0^{\pi/2} dx \frac{\cos^2 x \cdot \sin^2 x}{[\alpha + \sin^2 x]^2} \cdot \frac{\exp[\beta\bar{\omega}_0 \sin x]}{[\exp[\beta\bar{\omega}_0 \sin x] - 1]^2}.$$

a) At high temperature, the approximation (5.9a) applied to (8.2) and the same procedure as that of Sect. 6 lead to

$$z \cdot \left. \frac{dF_q(z)}{dz} \right|_{z=v_{\text{II}}|q|} \simeq -\frac{\Theta}{\alpha\gamma^2} \cdot \sqrt{\frac{\alpha+1}{\alpha}}.$$

Substitution of (6.3') gives the desired expression (for γ see eq. (9.1))

$$(8.3) \quad \left(\frac{dF_q(z)}{dz} \Big|_{z=v_{II}|q|} \right)^{-1} \simeq - \frac{v_{II}|q|\Theta^2}{(\gamma^2 + \Theta)(\gamma^2 + 2\Theta)}.$$

b) At low temperatures, (8.2) evaluated with the approximation (5.9b) takes the form

$$\begin{aligned} z \cdot \frac{dF_q(z)}{dz} \Big|_{z=v_{II}|q|} &\simeq - \frac{4\Theta}{\pi\gamma^2} \cdot \frac{\alpha+1}{\beta\bar{\omega}_0} \int_0^{\beta\bar{\omega}_0} \frac{dy}{(\alpha + (y/\beta\bar{\omega}_0)^2)^2} \cdot \frac{y^2 \exp[y]}{(\exp[y]-1)^2} = \\ &= - \frac{4\Theta}{\pi\gamma^2} \cdot \frac{\alpha+1}{\alpha} \cdot \frac{1}{\beta\bar{\omega}_0} \int_0^{\beta\bar{\omega}_0} \frac{dy}{\alpha + (y/\beta\bar{\omega}_0)^2} \cdot \frac{y^2 \exp[y]}{(\exp[y]-1)^2} + \\ &\quad + \frac{4\Theta}{\pi\gamma^2} \cdot \frac{\alpha+1}{\alpha} \cdot \left(\frac{1}{\beta\bar{\omega}_0} \right)^3 \int_0^{\beta\bar{\omega}_0} \frac{dy}{(\alpha + (y/\beta\bar{\omega}_0)^2)^2} \cdot \frac{y^4 \exp[y]}{(\exp[y]-1)^2}. \end{aligned}$$

Comparison with (7.1) and use of (4.6) shows that the first term equals

$$-2 \frac{\alpha+1}{\alpha} F_q(v_{II}|q|) = -2 \frac{\alpha+1}{\alpha}.$$

The second term is approximated by the method used in Sect. 7 and becomes

$$\begin{aligned} \frac{4\Theta}{\pi\gamma^2} \cdot \frac{\alpha+1}{\alpha} \cdot \left(\frac{1}{\beta\bar{\omega}_0} \right)^3 &\left\{ \frac{1}{\alpha^2} \int_0^{\gamma\bar{\alpha}\beta\bar{\omega}_0} dy \frac{y^4 \exp[y]}{(\exp[y]-1)^2} + (\beta\bar{\omega}_0)^4 \int_{\gamma\bar{\alpha}\beta\bar{\omega}_0}^{\beta\bar{\omega}_0} dy \frac{\exp[y]}{(\exp[y]-1)^2} \right\} = \\ &= \frac{4\Theta}{\pi\gamma^2} \cdot \frac{\alpha+1}{\alpha} \left(\frac{1}{\beta\bar{\omega}_0} \right)^3 \left\{ \frac{1}{\alpha^2} \int_0^{\gamma\bar{\alpha}\beta\bar{\omega}_0} \frac{y^3 dy}{\exp[y]-1} - \frac{(\beta\bar{\omega}_0)^4}{\exp[\sqrt{\alpha}\beta\bar{\omega}_0-1]} + \right. \\ &\quad \left. + (\beta\bar{\omega}_0)^4 \left(\frac{1}{\exp[\sqrt{\alpha}\beta\bar{\omega}_0]-1} - \frac{1}{\exp[\beta\bar{\omega}_0]-1} \right) \right\}. \end{aligned}$$

For consistency with (5.9b) the term of order $\beta\bar{\omega}_0/(\exp[\beta\bar{\omega}_0]-1)$ has to be neglected, and we have with $\Theta = \lambda\omega_0/\beta\omega_0$, $\bar{\omega}_0 = \gamma\omega_0$

$$z \frac{dF_q(z)}{dz} \Big|_{z=v_{II}|q|} \simeq -2 \frac{\alpha+1}{\alpha} \left(1 - \frac{8\lambda\omega_0}{\pi\gamma^5\alpha^2(\beta\omega_0)^4} \int_0^{\gamma\bar{\alpha}\gamma\beta\omega_0} \frac{y^3 dy}{\exp[y]-1} \right)$$

and

$$(8.4) \quad \left(\frac{dF_q(z)}{dz} \Big|_{z=v_{II}|q|} \right)^{-1} \simeq - \frac{\alpha v_{II}|q|}{2(\alpha+1)} \left(1 - \frac{8\lambda\omega_0}{3\pi\gamma^2\sqrt{\alpha}\beta\omega_0} \cdot \frac{3}{(\sqrt{\alpha}\gamma\beta\omega_0)^3} \int_0^{\gamma\bar{\alpha}\gamma\beta\omega_0} \frac{y^3 dy}{\exp[y]-1} \right)^{-1},$$

where γ and α have to be calculated from (9.2), (10.2) and Table 27.1 of ref. (12) may be used for the integral.

9. - The phonon renormalization factor γ .

The renormalization of the phonon frequencies (3.11) is determined by the solution of eq. (3.12)

$$\gamma^2 - \gamma - \Theta J(\gamma \cdot \beta \omega_0) = 0.$$

a) At high and intermediate temperatures, $J(\gamma \cdot \beta \omega_0)$ is given by (6.6). The rapid convergence of the series enables us to neglect terms with $n \geq 2$, so that we are left with a quadratic equation for γ in terms of the variables $u = \lambda \omega_0$ and $T/T_D = (\beta \omega_0)^{-1}$, with the solution

$$(9.1) \quad \gamma \simeq \frac{T}{T_D} \cdot \frac{12}{24(T/T_D) - u} \left\{ \left(1 - \frac{u}{\pi} \right) + \sqrt{\left(1 - \frac{u}{\pi} \right)^2 + 2u \frac{24(T/T_D) - u}{12}} \right\}.$$

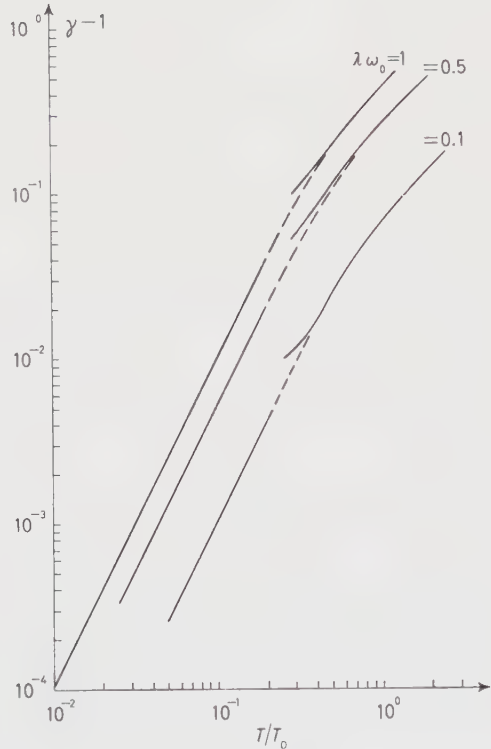
b) At low temperatures, $J(\gamma \cdot \beta \omega_0)$ is given by (7.8). In terms of the variables u and T/T_D γ will be the real solution of the cubic equation

$$\gamma^3 - \gamma^2 - \frac{\pi u}{3} \left(\frac{T}{T_D} \right)^2 = 0.$$

Hence

$$(9.2) \quad \gamma = 1 + 12^{-\frac{1}{2}} \cdot \left(\left[\sqrt{\pi u \left(\frac{T}{T_D} \right)^2 + \frac{4}{9}} + \frac{T}{T_D} \sqrt{\pi u} \right]^{\frac{1}{2}} - \left[\sqrt{\pi u \left(\frac{T}{T_D} \right)^2 + \frac{4}{9}} - \frac{T}{T_D} \sqrt{\pi u} \right]^{\frac{1}{2}} \right)^2.$$

Fig. 3. - The renormalization of the sound velocity $v_I/v_I^0 - 1 \equiv \gamma - 1$ vs. T/T_D for three values of the anharmonic coupling parameter $\lambda \cdot \omega_0$.



For $(T/T_D)\sqrt{\pi u} \ll 1$ this simplifies to

$$(9.2') \quad \gamma \simeq 1 + \frac{\pi u}{3} \left(\frac{T}{T_D} \right)^2.$$

For temperatures $10^{-2} \leq T/T_D \leq 2.5$ and $u = 10^{-1}$, $5 \cdot 10^{-1}$ and 1 , $(\gamma - 1)$ is shown graphically in Fig. 3.

10. - The eigenvalue α .

a) At high and intermediate temperatures, α is given by (6.3'), which in terms of the variables u and T/T_D reads

$$(10.1) \quad \alpha = \frac{u^2 (T/T_D)^2}{\gamma^2 (\gamma^2 + 2u(T/T_D))}.$$

Here the values of γ taken from (9.1) have to be substituted.

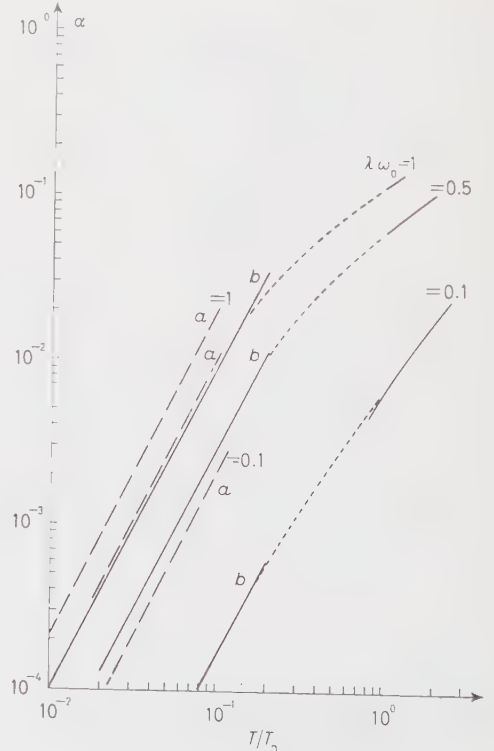
b) At low temperatures α is given by (7.7). For $|u/\gamma| \ll 1$ only the upper sign of the root in (7.7) is compatible with the condition for (6.5), $|\sqrt{\alpha}\gamma|T_D/T < 2\pi$. To lowest order in u/γ one then finds

$$(10.2) \quad \alpha \simeq \left(\frac{4u}{\pi\gamma^2} \cdot \frac{T}{T_D} \right)^2.$$

For computation, the values of γ taken either from (9.2) or (9.2') have to be substituted. To illustrate the error resulting from the crude approximation, which led to the expression (7.2) for α

$$(10.3) \quad \alpha \simeq \frac{2\pi}{3\gamma^3} \cdot u \cdot \left(\frac{T}{T_D} \right)^2,$$

Fig. 4. - The eigenvalue $\alpha \equiv (v_{II}/v_I)^2 - 1$ vs. T/T_D for three values of the anharmonic coupling parameter $\lambda \cdot \omega_0$. a) α calculated from (10.3), b) α calculated from (10.1) and (10.2), for $\lambda\omega_0 = 0.1$, from (10.1) and (7.7), for $\lambda\omega_0 = 0.5$ and 1.0 .



both curves for α , the one resulting from (10.2) or (7.7) and the other from (10.3) are reported in Fig. 4, where the remark below (7.1) becomes evident.

11. – Collective-mode propagator.

In analogy to the one-phonon propagator (3.3) a propagator of the collective mode may be defined as

$$(11.1) \quad \mathbf{G}(q, \tau) \equiv \langle T \{ c_q(\tau) c_q^*(0) \} \rangle .$$

Through (4.1) this propagator is related to the correlation function ⁽¹³⁾

$$(11.2) \quad C_{k,k'}(q, \tau) = \langle T \{ \delta n_k(-q, \tau) \delta n_{k'}(q, 0) \} \rangle ,$$

where $n_k(q)$ is given by (2.2') and $\delta A \equiv A - \langle A \rangle$.

Indeed, for $q \neq 0$ and in the same approximation as (2.3'), *i.e.* neglecting Umklapp (momentum conservation) and with

$$(11.3) \quad \begin{aligned} \langle n_k(q) \rangle &\simeq \delta_{q,0} n_k , \\ \mathbf{G}(q, \tau) &= \sum_{k,k'} \alpha_{k+q,k} \alpha_{k',k'-q}^* C_{k,k'}(q, \tau) . \end{aligned}$$

On the other hand, $C_{k,k'}(q, \tau)$ is the two-phonon Green's function

$$(11.4) \quad K \left(\begin{array}{cc} k, \tau; & k', \tau' \\ k+q, \mu; & k'-q, \mu' \end{array} \right) = \langle T \{ \delta(b_k^*(\tau) b_{k+q}(\mu)) \delta(b_{k'}^*(\tau') b_{k'-q}(\mu')) \} \rangle$$

taken at $\mu = \tau$ and $\mu' = \tau' = 0$.

Between the Fourier transforms

$$(11.2') \quad \tilde{C}_{k,k'}(q, i\nu) = \int_{\square}^{\beta} d\tau \exp[-i\nu\tau] C_{k,k'}(q, \tau) ,$$

$$(11.4') \quad \begin{aligned} \tilde{K} \left(\begin{array}{cc} k, i\sigma; & k', i\sigma' \\ k+q, i(\sigma+\nu); & k'-q, i(\sigma'-\nu') \end{array} \right) = \\ = \int_0^{\beta} d\tau \exp[i\sigma\tau] \int_0^{\beta} d\mu \exp[-i(\sigma+\nu)\mu] \int_0^{\beta} d\tau' \exp[i\sigma'\tau'] \int_0^{\beta} d\mu' \exp[-i(\sigma'-\nu')\mu'] \otimes \\ \otimes K \left(\begin{array}{cc} k, \tau; & k', \tau' \\ k+q, \mu; & k'-q, \mu' \end{array} \right) = \end{aligned}$$

⁽¹³⁾ C. P. ENZ: in *Theory of Condensed Matter, International Center for Theoretical Physics, Trieste, 1967, IAEA* (Vienna, 1968), p. 762.

The importance of the linear chain model now is that according to (2.8) $\tau_{(k, k'+q)(-k-q, -k')}$ factorizes ⁽²⁾. Graphically

$$(11.11) \quad -\frac{1}{3!} \tau_{(k, k'+q)(-k-q, -k')} = \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k'' \\ \curvearrowright \\ k''+q \end{array},$$

or with (2.8)

$$(11.11') \quad \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} = \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} = i \sqrt{\frac{\lambda}{N}} \cdot \sqrt{\omega_k \omega_{k+q}},$$

so that (11.9) reads

$$(11.12) \quad \begin{array}{c} k \quad k'-q \\ \curvearrowright \\ k+q \quad k' \end{array} \cong \delta_{k', k+q} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} + \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k'' \\ \curvearrowright \\ k''+q \end{array} \begin{array}{c} k' \\ \curvearrowright \\ k' \end{array}.$$

If we define in addition

$$(11.13) \quad \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} = \alpha_{k+q, k}; \quad \begin{array}{c} k-q \\ \curvearrowright \\ k \end{array} = \alpha_{k, k-q}^*,$$

then we obtain from (11.3) and (11.12)

$$(11.14) \quad \tilde{\mathbf{G}}(q, z) = \begin{array}{c} \curvearrowright \\ \curvearrowright \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k'-q \\ \curvearrowright \\ k' \end{array} = \begin{array}{c} \curvearrowright \\ \curvearrowright \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} + \begin{array}{c} \curvearrowright \\ \curvearrowright \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k'' \\ \curvearrowright \\ k''+q \end{array} \begin{array}{c} k' \\ \curvearrowright \\ k' \end{array}.$$

This introduces the additional function

$$(11.15) \quad \tilde{\mathbf{F}}(q, z) \equiv i \sqrt{\frac{\lambda}{N}} \sum_{k, k'} \sqrt{\omega_k \omega_{k+q}} \tilde{\mathbf{C}}_{k, k'}(q, z) \alpha_{k', k'-q}^* = \begin{array}{c} \curvearrowright \\ \curvearrowright \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k'-q \\ \curvearrowright \\ k' \end{array}.$$

for which the equation

$$(11.16) \quad \begin{array}{c} \curvearrowright \\ \curvearrowright \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k'-q \\ \curvearrowright \\ k' \end{array} = \begin{array}{c} \curvearrowright \\ \curvearrowright \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} + \begin{array}{c} \curvearrowright \\ \curvearrowright \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k'' \\ \curvearrowright \\ k''+q \end{array} \begin{array}{c} k' \\ \curvearrowright \\ k' \end{array}.$$

follows from (11.12). Now (11.14) and (11.16) yield

$$(11.17) \quad \tilde{\mathbf{G}}(q, z) = \begin{array}{c} \curvearrowright \\ \curvearrowright \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k'-q \\ \curvearrowright \\ k' \end{array} + \left(\begin{array}{c} \curvearrowright \\ \curvearrowright \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k'' \\ \curvearrowright \\ k''+q \end{array} \begin{array}{c} k' \\ \curvearrowright \\ k' \end{array} \right) / \left(1 - \begin{array}{c} \curvearrowright \\ \curvearrowright \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \begin{array}{c} k \\ \curvearrowright \\ k+q \end{array} \right).$$

With (3.9) the Lindhard function becomes

$$(11.18) \quad \tilde{L}_k(q, z) = \frac{\bar{n}_k - \bar{n}_{k+q}}{z - (\bar{\omega}_k - \bar{\omega}_{k+q})}$$

and with (11.11') and (4.6')

$$(11.19) \quad \text{Diagram: a circle labeled } L \text{ with two horizontal lines passing through it, each ending in a semi-circle} = F_q(z) .$$

Making use of (4.5) and (4.7) we also find

$$(11.20) \quad \text{Diagram: a circle labeled } L \text{ with two horizontal lines passing through it, each ending in a triangle pointing outwards} = |N_q|^2 \cdot \frac{N}{\lambda} \cdot \frac{1}{z + \Omega_q} \left\{ \frac{1 - F_q(z)}{z + \Omega_q} + \frac{\lambda}{N \cdot |N_q|^2} \right\} ,$$

$$(11.21) \quad \text{Diagram: a circle labeled } L \text{ with two horizontal lines passing through it, each ending in a semi-circle} = \frac{N_q}{N_q^*} \text{Diagram: a circle labeled } L \text{ with two horizontal lines passing through it, each ending in a triangle pointing outwards} = iN_q \sqrt{\frac{N}{\lambda}} \cdot \frac{1 - F_q(z)}{z + \Omega_q} .$$

Substitution of (11.19), (11.20) and (11.21) into (11.17) finally gives

$$(11.22) \quad \tilde{\mathbf{G}}(q, z) = \frac{1}{\Omega_q + z} .$$

Quite generally a pole of a propagator may be put in evidence by writing ⁽¹³⁾

$$(11.23) \quad \tilde{\mathbf{G}}(q, z) = \frac{z_q}{\Omega_q + z} + \tilde{\mathbf{G}}_{\text{reg}}(q, z) ,$$

where z_q is the wave function renormalization factor. The fact that the regular part $\tilde{\mathbf{G}}_{\text{reg}}(q, z)$ is missing in (11.22) and that $z_q = 1$ is due to the approximations we made. Thus if an external source couples to c_q , in this approximation the collective mode is excited completely.

From (4.1) and (4.5) one sees that c_q is a density operator very similar to the energy density ^(2,6) and hence is expected to couple to a local temperature variation, whereas the phonon operator $b_q + b_{-q}^*$ couples to a local force. In order to find the amplitude of this coupling the residue of the collective-mode pole in the energy-density autocorrelation function ⁽⁶⁾ would have to be calculated, in analogy to the calculation of SHAM ⁽¹⁴⁾ for the hydrodynamic domain where the analogue to the collective mode is second sound.

The collective-mode density

$$(11.24) \quad \mathbf{N}(q) = \langle c_q^* c_q \rangle = \beta^{-1} \sum_{\sigma} \tilde{\mathbf{G}}(q, i\sigma)$$

⁽¹⁴⁾ L. J. SHAM: *Phys. Rev.*, **156**, 494 (1967); **163**, 401 (1967).

is obtained exactly in the same way as for phonons and turns out to be the Bose distribution

$$(11.25) \quad \mathbb{N}(q) = (\exp [\beta \Omega_q] - 1)^{-1}.$$

12. – Conclusions.

From the fact, that the simple formalism used here leads to a real renormalization of the phonon frequency ω_k (Sect. 3), it is obvious that the results lose their validity as soon as the renormalization factor $\gamma(\lambda, T)$ appreciably exceeds 1, because then the damping of the phonons becomes important.

In the region of applicability of this formalism, $0 \leq T/T_D < 1$ and $0 \leq \lambda\omega_0 \leq 1$, the eigenvalue $\alpha = (v_{II}/v_I)^2 - 1$ is seen from Fig. 4 to be less than 10^{-1} . We may then write

$$(12.1) \quad v_{II} = \sqrt{\alpha + 1} v_I \simeq v_I \cdot \left(1 + \frac{\alpha}{2}\right) \equiv v_I + \Delta v_{II}.$$

For $\lambda\omega_0 = 10^{-1}$ we have

$$(12.2) \quad 0 \leq \frac{\Delta v_{II}}{v_I} \leq 10^{-2}$$

and for $\lambda\omega_0 = 1$

$$(12.2') \quad 0 \leq \frac{\Delta v_{II}}{v_I} \leq 6 \cdot 10^{-2}.$$

If we compare this to

$$(12.3) \quad \Delta v_I \equiv v_I - v_I^0 = v_I^0(\gamma - 1)$$

the difference between the renormalized and the unrenormalized sound velocity, we find

$$(12.4) \quad \frac{\Delta v_{II}}{\Delta v_I} = \frac{\gamma(\sqrt{\alpha + 1} - 1)}{\gamma - 1}$$

shown graphically in Fig. 5. There, one sees that

$$(12.5) \quad 4 \cdot 10^{-2} < \frac{\Delta v_{II}}{\Delta v_I} < 5 \cdot 10^{-1},$$

so that the difference between the collective sound and the ordinary sound is almost of the same order of magnitude as the renormalization of ordinary sound.

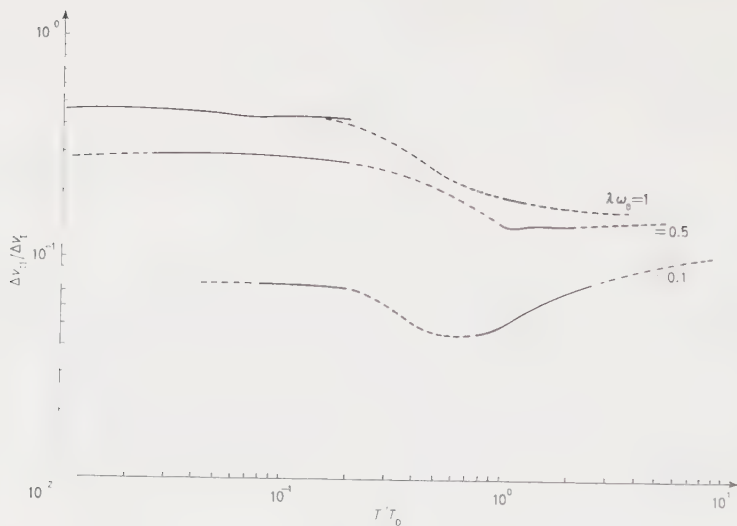


Fig. 5. — Plot of $(v_{II} - v_I)/(v_I - v_I^0)$, where v_I^0 is the sound velocity in the absence of anharmonic effects, v_I is the sound velocity as corrected for anharmonic effects and v_{II} is the velocity of the collective mode.

In order to answer the question, whether the collective-sound mode is observable, the residue of the collective-mode pole mentioned at the end of Sect. 11 would have to be compared to the residue of the phonon pole, and this as well for elastic as for thermal external coupling. In the calculation of these quantities, the damping of the phonons and *a fortiori* the phonon number non-conserving interactions, will play an important role. The study of the effect of phonon nonconservation on the collective mode within the scheme of this theory will be the subject of Part II.

APPENDIX A

Definition of the coefficients of $\tilde{H}$.

$$4\mu_{(k_1, \dots, k_4)} \equiv C_{k_1, \dots, k_4}^{(4)} + B_{(k_1, \dots, k_4)}^{(4)},$$

$$4\nu_{k_1(k_2, k_3, k_4)} \equiv 4C_{k_1, \dots, k_4}^{(4)} + B_{k_1(k_2, k_3, k_4)}^{(3)},$$

$$4\tau_{(k_1, k_2)(k_3, k_4)} \equiv 6C_{k_1, \dots, k_4}^{(4)} + B_{(k_1, k_2)(k_3, k_4)}^{(2)},$$

$$\lambda_k = \frac{3}{2 \cdot 4!} \sum_{k'} \left\{ C_{k', -k', -k, k}^{(4)} - \frac{1}{2} \sum_{k''} |C_{k, k', k''}^{(3)}|^2 \left(\frac{1}{\omega_k + \omega_{k'} + \omega_{k''} + i\varepsilon} + \frac{1}{\omega_k + \omega_{k'} - \omega_{k''} - i\varepsilon} \right) \right\},$$

$$B_{(k_1, k_2, k_3, k_4)}^{(4)} \equiv -\frac{3}{2} S_{k_1 k_2 k_3 k_4} \sum_q C_{k_1, k_2, q}^{(3)} C_{k_3, k_4, -q}^{(3)} \cdot \left(\frac{\omega_q}{\omega_q^2 - (\omega_{k_1} + \omega_{k_2} + i\varepsilon)^2} + \frac{\omega_q}{\omega_q^2 - (\omega_{k_3} + \omega_{k_4} + i\varepsilon)^2} \right),$$

$$B_{(k_1, k_2, k_3, k_4)}^{(3)} \equiv -6 S_{k_2 k_3 k_4} \sum_q C_{k_1, k_2, q}^{(3)} C_{k_3, k_4, -q}^{(3)} \cdot \left(\frac{\omega_q}{\omega_q^2 - (\omega_{k_2} - \omega_{k_1} + i\varepsilon)^2} + \frac{\omega_q}{\omega_q^2 - (\omega_{k_3} + \omega_{k_4} + i\varepsilon)^2} \right),$$

$$B_{(k_1, k_2)(k_3, k_4)}^{(2)} \equiv -3 \sum_q C_{k_1, k_2, q}^{(3)} C_{k_3, k_4, -q}^{(3)} \left(\frac{\omega_q}{\omega_q^2 - (\omega_{k_1} + \omega_{k_2} + i\varepsilon)^2} + \frac{\omega_q}{\omega_q^2 - (\omega_{k_3} + \omega_{k_4} + i\varepsilon)^2} \right) - 6 S_{k_3 k_4} \sum_q C_{k_1, k_2, q}^{(3)} C_{k_3, k_4, -q}^{(3)} \left(\frac{\omega_q}{\omega_q^2 - (\omega_{k_3} - \omega_{k_1} + i\varepsilon)^2} + \frac{\omega_q}{\omega_q^2 - (\omega_{k_4} - \omega_{k_2} + i\varepsilon)^2} \right).$$

Here $S_{k_1, \dots, k_n}$ is the symmetrization operator defined by

$$S_{k_1, \dots, k_n} f(k_1, \dots, k_n) = \frac{1}{n!} \sum_{\substack{\text{all permutations} \\ P(k_1, \dots, k_n)}} f(P(k_1, \dots, k_n)),$$

$$\tilde{E}_0 = E_0 + \frac{3}{4 \cdot 4!} \sum_{k, k'} C_{k', -k', k, -k}^{(4)} - \frac{1}{2 \cdot 4!} \sum_{k_1 k_2 k_3} \frac{|C_{k_1, k_2, k_3}^{(3)}|^2}{\omega_{k_1} + \omega_{k_2} + \omega_{k_3}}.$$

APPENDIX B

Dynamics of a monatomic linear chain with nearest-neighbour interactions.

Let us denote the position of the n -th atom by $x_n = n \cdot a + u_n$ where a is the inter-atomic spacing at equilibrium and the periodic boundary condition $u_{N+1} = u_1$ is used. The Hamiltonian for the chain with nearest-neighbour interactions is

$$H = \sum_{n=1}^N \left\{ \frac{m}{2} \left(\frac{\partial u_n}{\partial t} \right)^2 + \varphi(|u_{n+1} - u_n + a|) \right\},$$

where $\varphi(r)$ is the two-body potential and m the mass of the atoms.

Then, following ref. ⁽¹⁵⁾, but denoting by k the one-dimensional wave vector $-\pi/a < k \leq \pi/a$ and using for the polarization vectors

$$e(k) = e^*(-k)$$

⁽¹⁵⁾ A. A. MARADUDIN, P. A. FLINN and R. A. COLDWELL-HORSFALL: *Ann. of Phys.*, **15**, 337 (1961).

in accordance with the definition (1.3), we get for H the form (1.1), where

$$(B.1) \quad \omega_k = \sqrt{\frac{4\lambda_2}{m}} \cdot \left| \sin \frac{ak}{2} \right| = \omega_0 \cdot \left| \sin \frac{ak}{2} \right|,$$

$$(B.2) \quad C_{k_1, \dots, k_n}^{(n)} = N^{-(n-2)/2} \cdot \lambda_n \cdot \lambda_2^{-n/2} \cdot \prod_{\nu=1}^n \{i\sigma(k_\nu) \cdot e(k_\nu) \cdot \omega_{k_\nu}^{\frac{1}{2}}\} \tilde{\Delta} \left(\sum_{i=1}^n k_i \right)$$

with $\sigma(k_\nu) \equiv \text{sign}(k_\nu)$ and $\lambda_\nu \equiv (d^{\nu} \varphi(r)/dr^{\nu})|_{r=a}$, and

$$(B.3) \quad \tilde{\Delta} \left(\sum_{i=1}^n k_i \right) \equiv \delta_{\sum_i k_i, 0} + \sum_{\nu=1}^n (-1)^{\nu} \left(\delta_{\sum_i k_i, \nu(2\pi/a)} + \delta_{\sum_i k_i, -\nu(2\pi/a)} \right).$$

The requirement that the atomic displacements in three dimensions ⁽⁶⁾

$$\mathbf{u}(\mathbf{R}, b; t) = \sum_{\mathbf{k}} (BG)^{-\frac{1}{2}} (M_b \omega_k)^{-\frac{1}{2}} \cdot \mathbf{e}_k(b) \exp[i\mathbf{k} \cdot \mathbf{R}] Q_k(t),$$

transform like real polar vectors under time-reversal and parity fixes the transformation properties of the product $\mathbf{e}_k(b)Q_k(t)$, leaving a choice for one of both factors, in particular axial or polar polarization vectors $\mathbf{e}_k(b)$.

For crystals with an inversion centre the invariance of the Hamiltonian (1.1) under parity implies that the anharmonic coefficients $C_{k_1, \dots, k_n}^{(n)}$ are

- i) real for n even, purely imaginary for n odd when $\mathbf{e}_k(b)$ is axial ⁽¹⁶⁾,
- ii) real for all n when $\mathbf{e}_k(b)$ is polar.

In the one-dimensional case considered here, the co-ordinate of $\mathbf{e}(k)$ is

$$\begin{aligned} e(k) &= \pm 1 && \text{in case i),} \\ e(k) &= \pm i \cdot \sigma(k) && \text{in case ii).} \end{aligned}$$

We use the second convention.

APPENDIX C

The coefficients $\tau_{(q-k_s-k')|(k_s k'-q)^*}$

According Appendix A, sums of the form

$$\Sigma \{f\} = \sum_l C_{k_1, k_2, l}^{(3)} C_{k_3 k_4, -l}^{(3)} f(\omega_l; \omega_{k_1}, \omega_{k_2}, \omega_{k_3}, \omega_{k_4})$$

⁽¹⁶⁾ I. P. IPATOVA, A. A. MARADUDIN and R. F. WALLIS: *Phys. Rev.*, **155**, 882 (1967).

have to be evaluated, where f is any algebraic function. In the case of the linear chain considered here the sum $\sum_l$ can be eliminated via crystal-momentum conservation.

As shown in Appendix B, $C_{k_1, k_2, l}^{(3)} = \bar{C}_{k_1, k_2, l} \cdot \tilde{\Delta}(k_1 + k_2 + l)$, which implies

$$\Sigma\{f\} = \tilde{\Delta}(k_1 + k_2 + k_3 + k_4) \sum_l \bar{C}_{k_1, k_2, l} \bar{C}_{k_3, k_4, -l} \Delta(k_1 + k_2 + l) f(\omega_l; \omega_{k_1}, \dots, \omega_{k_4})$$

where

$$\Delta\left(\sum_i k_i\right) = \begin{cases} 1 & \text{if } \sum_i k_i = \nu \cdot \frac{2\pi}{a}, \quad \nu = 0, \pm 1, \pm 2, \dots, \\ 0 & \text{otherwise,} \end{cases}$$

with

$$\omega_{k+p \cdot 2\pi/a} = \omega_k$$

and

$$\bar{C}_{k_1, k_2, l} = N^{-\frac{1}{2}} \cdot \lambda_3 \cdot \lambda_2^{-\frac{1}{2}} \cdot (\omega_{k_1} \cdot \omega_{k_2} \cdot \omega_l)^{\frac{1}{2}}$$

follows

$$\Sigma\{f\} = N^{-1} \cdot \lambda_3^2 \cdot \lambda_2^{-3} (\omega_{k_1} \cdot \omega_{k_2} \cdot \omega_{k_3} \cdot \omega_{k_4})^{\frac{1}{2}} \tilde{\Delta}\left(\sum_{i=1}^4 k_i\right) \cdot \omega_{k_1+k_2} \cdot f(\omega_{k_1+k_2}; \omega_{k_1}, \dots, \omega_{k_4}) \cdot \sum_l \Delta(k_1 + k_2 + l).$$

Because k_1, k_2 and l are within the 1st Brillouin zone $\sum_l \Delta(k_1 + k_2 + l) = 1$. This rule applied to $B_{(k, p-q)(-p, q-k)}^{(2)}$ gives

$$\begin{aligned} & -\frac{3}{2} N^{-1} \cdot \lambda_3^2 \cdot \lambda_2^{-3} \cdot (\omega_k \cdot \omega_{k-q} \cdot \omega_p \cdot \omega_{p-q})^{\frac{1}{2}} \cdot \\ & \cdot \left\{ \frac{2\omega_{k+p-q}^2}{\omega_{k+p-q}^2 - (\omega_k + \omega_{p-q} - i\varepsilon)^2} + \frac{2\omega_{k+p-q}^2}{\omega_{k+p-q}^2 - (\omega_p + \omega_{k-q} + i\varepsilon)^2} + \right. \\ & + \frac{2\omega_{k-p}^2}{\omega_{k-p}^2 - (\omega_p - \omega_k + i\varepsilon)^2} + \frac{2\omega_{k-p}^2}{\omega_{k-p}^2 - (\omega_{p-q} - \omega_{k-q} - i\varepsilon)^2} + \\ & \left. + \frac{2\omega_q^2}{\omega_q^2 - (\omega_{k-q} - \omega_k + i\varepsilon)^2} + \frac{2\omega_q^2}{\omega_q^2 - (\omega_{q-p} - \omega_p - i\varepsilon)^2} \right\}. \end{aligned}$$

If we denote the parenthesis by $4\beta_{k,p}(q)$, we have together with $C_{k, p-q, -p, q-k}^{(4)}$

$$4\tau_{(k, p-q)(-p, q-k)} = 6N^{-1} \sqrt{\omega_k \cdot \omega_{k-q} \cdot \omega_p \cdot \omega_{p-q}} \left(\frac{\lambda_4}{\lambda_2^2} - \frac{\lambda_3^2}{\lambda_2^3} \cdot \beta_{k,p}(q) \right).$$

Because $\lambda_4 \cdot \lambda_2$ is of the same order of magnitude as λ_3^2 the limit $q \rightarrow 0$ may be taken for $\beta_{k,p}(q)$. With $\omega_k = \omega_0 |\sin(ak/2)|$ it turns out that $\lim_{q \rightarrow 0} \beta_{k,p}(q) = 1$. The definition of a coupling constant $4\lambda = (\lambda_4 \lambda_2 - \lambda_3^2) \lambda_2^{-3}$ which has the dimension of an inverse energy leads to (2.8).

PART II.

Introduction.

In part I we established the existence of a soundlike collective mode in a monatomic linear chain and calculated its energy for long wavelengths in RPA neglecting phonon-number-nonconserving interactions in the Hamiltonian.

The effect of these interactions on the energy of the collective mode for temperatures $T \ll T_D$ and for weak coupling $\lambda\omega_0 \ll 1$ is analysed in the present part II. It will turn out that the omission in I of the nonconserving interactions was justified, in spite of the fact that they are of the same order in the coupling parameter λ (defined in Appendix I C) as the phonon number-conserving interactions.

The renormalization of the phonon frequencies which entered the calculation of the collective velocity was evaluated in I in the same approximation as the collective mode. For keeping this consistency, we start by deriving the phonon propagators in RPA when the number of phonons is not conserved.

1. -- Phonon propagators in RPA.

Up to order $O[|u/r_0|^3]$, where u is an average atomic displacement and r_0 the nearest-neighbour spacing, the normal order of the Hamiltonian describing the phonon system follows from (I-1.7)

$$\begin{aligned}
 (1.1) \quad :\tilde{H}: &= \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^* b_{\mathbf{k}} + \frac{1}{4!} \sum_{\mathbf{k}_1 \dots \mathbf{k}_4} \tau_{(\mathbf{k}_1, \mathbf{k}_2)(\mathbf{k}_3, \mathbf{k}_4)} b_{-\mathbf{k}_1}^* b_{-\mathbf{k}_2}^* b_{\mathbf{k}_3} b_{\mathbf{k}_4} + \\
 &+ \frac{1}{4!} \sum_{\mathbf{k}_1 \dots \mathbf{k}_4} \{ (\mu_{(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4)} b_{\mathbf{k}_1} b_{\mathbf{k}_2} b_{\mathbf{k}_3} b_{\mathbf{k}_4} + \text{h.c.}) + (\nu_{\mathbf{k}_1(\mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4)} b_{-\mathbf{k}_1}^* b_{\mathbf{k}_2} b_{\mathbf{k}_3} b_{\mathbf{k}_4} + \text{h.c.}) \}.
 \end{aligned}$$

tension of eq. (I-3.5) with the phonon number-nonconserving vertex T , assuming momentum conservation, *i.e.*

$$\int_0^\beta d\tau \exp[-i\sigma\tau] \langle T \{ b_k(\tau) b_{k'}^*(0) \} \rangle \simeq \delta_{k,k'} \tilde{g}(k, i\sigma),$$

$$\int_0^\beta d\tau \exp[-i\sigma\tau] \langle T \{ b_k(\tau) b_{-k}(0) \} \rangle \simeq \delta_{k,k'} \tilde{g}_1(k, i\sigma).$$

RPA consists in taking Σ and T , which are defined through eqs. (1.4a) and (1.4b) to lowest order in the interaction:

$$(1.5) \quad \Sigma(k, \sigma) = \text{diagram of a circle with } \Sigma \text{ in the center and } k \text{ on both sides} \simeq \beta^{-1} \sum_{l, \sigma'} \text{diagram of a ring with a square } \tau \text{ on top and } k \text{ on both sides, labeled } (l, \sigma') ,$$

$$(1.6a) \quad T(k, \sigma) = \text{diagram of a circle with } T \text{ in the center, } -k \text{ on the left and } k \text{ on the right} \simeq \beta^{-1} \sum_{l, \sigma'} \text{diagram of a ring with a square } \nu \text{ on top, } -k \text{ on the left and } k \text{ on the right, labeled } (l, \sigma') ,$$

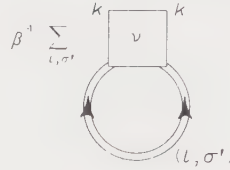
$$(1.6b) \quad T^*(k, \sigma) = \text{diagram of a circle with } T^* \text{ in the center, } k \text{ on the left and } -k \text{ on the right} \simeq \beta^{-1} \sum_{l, \sigma'} \text{diagram of a ring with a square } \nu^* \text{ on top, } k \text{ on the left and } -k \text{ on the right, labeled } (l, \sigma') ,$$

where the momentum-conserving 4-phonon vertices are

$$(1.7) \quad \text{diagram of a square } \tau \text{ with } q \text{ on top-left, } p \text{ on top-right, } q-l \text{ on bottom-left, and } p-l \text{ on bottom-right} = -\frac{1}{3!} \tau_{(-p, l-q)(q, p-l)},$$

$$(1.8) \quad \text{diagram of a square } \nu^* \text{ with } -q \text{ on top-left, } p \text{ on top-right, } q-l \text{ on bottom-left, and } p-l \text{ on bottom-right} = -\frac{3!}{4!} \nu_{l-p(p, -q, q-l)}^*.$$

One may be tempted to include in (1.5) terms like



but since (1.4b) contains no inhomogeneous part (in opposition to (1.4a)), terms of this kind are one order higher in the interaction than (1.5).

The phonon distribution is related to the propagator $\tilde{g}(k, i\sigma)$ by (I-3.7)

$$(1.9) \quad \beta^{-1} \sum_{\sigma} \tilde{g}(k, i\sigma) = n_k,$$

where

$$(1.10) \quad n_k \equiv \langle n_k(0) \rangle$$

and (I-2.2')

$$(1.11) \quad n_k(q) \equiv b_k^* b_{k-q}$$

and the average is defined in (1.3).

Substitution of (1.7) into (1.5) and (1.8) into (1.6), respectively gives, together with (1.9),

$$(1.5') \quad \Sigma(k) = -\frac{1}{3!} \sum_{k'} \tau_{(-k, -k') (k', k)} n_{k'},$$

$$(1.6') \quad T(k) = -\frac{1}{4} \sum_{k'} v_{-k' (k, -k, k')} n_{k'}.$$

With (I-2.8) we have

$$(1.7') \quad \tau_{(-k, -k') (k', k)} = 3! \frac{\lambda}{N} \omega_k \omega_{k'}.$$

Then $\omega_{-k} = \omega_k$ and the symmetry of $v_{-k' (k, -k, k')}$ with respect to interchanging k and $(-k)$ imply

$$(1.5'') \quad \Sigma(-k) = \Sigma(k)$$

and

$$(1.6'') \quad T(-k) = T(k).$$

Because in the structure equations (1.4) all summations over internal variables are contained within $\Sigma(k)$ and $T(k)$, the solution is purely algebraic.

From (1.4b) we get

$$(1.12) \quad \tilde{g}_1(k, i\sigma) = \frac{T^*(k)}{[\tilde{g}^0(-k, -i\sigma)]^{-1} - \Sigma(k)} \cdot \tilde{g}(k, i\sigma).$$

Substitution into (1.4a) gives for the main phonon propagator

$$\tilde{g}(k, i\sigma) = \left([\tilde{g}^0(k, i\sigma)]^{-1} - \Sigma(k) - \frac{|T(k)|^2}{[\tilde{g}^0(-k, -i\sigma)]^{-1} - \Sigma(k)} \right)^{-1}.$$

With $[\tilde{g}^0(k, i\sigma)]^{-1} = \omega_k + i\sigma$ (I-3.4), $\omega_k = \omega_{-k}$ and (1.5''), (1.6'') we obtain

$$(1.13) \quad \tilde{g}(k, i\sigma) = \tilde{g}(-k, i\sigma) = \frac{\omega_k - \Sigma(k) - i\sigma}{(\omega_k - \Sigma(k))^2 - |T(k)|^2 + \sigma^2}.$$

The usual form for a propagating quasi-particle is obtained by combining

$$(1.14) \quad \frac{1}{|\alpha_k|^2 + |\beta_k|^2} (|\beta_k|^2 \tilde{g}(k, i\sigma) - |\alpha_k|^2 \tilde{g}(k, -i\sigma)) \equiv \tilde{G}(k, i\sigma),$$

where

$$(1.15) \quad \begin{cases} |\alpha_k|^2 = \frac{1}{2} [(\omega_k - \Sigma(k))((\omega_k - \Sigma(k))^2 - |T(k)|^2)^{-\frac{1}{2}} - 1], \\ |\beta_k|^2 = \frac{1}{2} [(\omega_k - \Sigma(k))((\omega_k - \Sigma(k))^2 - |T(k)|^2)^{-\frac{1}{2}} + 1]. \end{cases}$$

Indeed, substitution of (1.13) and (1.15) into (1.14) leads to

$$(1.16) \quad \tilde{G}(k, i\sigma) = \tilde{G}(-k, i\sigma) = \frac{1}{\sqrt{(\omega_k - \Sigma(k))^2 - |T(k)|^2 + i\sigma}}.$$

2. - The quasi-phonon in RPA.

The function $\tilde{G}(k, i\sigma)$ describes the propagation of a quasi-phonon with energy

$$(2.1) \quad \hat{\omega}_k = \sqrt{(\omega_k - \Sigma(k))^2 - |T(k)|^2}.$$

The easiest way of seeing how this quasi-phonon is related to the phonon operators consists in applying RPA to the Hamiltonian (1.1) in the operator form (I-2.3). The result is

$$:\tilde{H}:_{\text{RPA}} = \sum_k \left\{ \left(\omega_k + \frac{1}{3!} \sum_{k'} \tau_{(k', -k)(k', k)} n_{k'} \right) b_k^* b_k + \left[\left(\frac{3}{4!} \sum_{k'} \tau_{-k'(k', k), (k, -k)} n_{k'} \right) b_k b_{-k} + \text{h.c.} \right] \right\}.$$

As in the previous Section, $n_{k'}$ is now defined by (1.10), (1.11) and (1.3). Now (1.5') and (1.6') allow us to write

$$(2.2) \quad :\tilde{H}:_{\text{RPA}} = \sum_k \{ (\omega_k - \Sigma(k)) b_k^* b_k - \frac{1}{2} (T(k) b_k b_{-k} + \text{h.c.}) \}.$$

The Hamiltonian (2.2) can be diagonalized via the Bogoliubov transformation

$$(2.3) \quad b_k = \alpha_k^* a_{-k}^* + \beta_k a_k,$$

where the new operator a_k is the annihilation operator of a quasi-phonon with momentum k .

Requiring the transformation to be canonical, we obtain from

$$(2.4) \quad [a_k, a_{k'}^*]_- = \delta_{k,k'},$$

$$(2.4') \quad |\beta_k|^2 - |\alpha_k|^2 = 1$$

and from

$$(2.5) \quad [a_k, a_{k'}]_- = 0,$$

$$(2.5') \quad \alpha_k^* \beta_{-k} = \alpha_{-k}^* \beta_k.$$

Here, the commutation relations

$$[b_k, b_{k'}^*]_- = \delta_{k,k'}, \quad [b_k, b_{k'}]_- = 0,$$

of the phonon operators have been used.

Then (2.4') and (2.5') also imply

$$(2.6) \quad |\alpha_k|^2 = |\alpha_{-k}|^2, \quad |\beta_k|^2 = |\beta_{-k}|^2, \quad \alpha_{-k} \beta_{-k} = \alpha_k \beta_k.$$

The substitution of (2.3) into (2.2) with use of (1.5''), (1.6'') and $\omega_k = \omega_{-k}$ gives the transformed Hamiltonian $\hat{H}$ in terms of the new operators,

$$\begin{aligned} \hat{H} = \sum_k \{ & [(\omega_k - \Sigma(k)) (|\beta_k|^2 + |\alpha_{-k}|^2) - (T(k) \beta_k \alpha_{-k}^* + \text{h.c.})] a_k^* a_k + \\ & + [(\omega_k - \Sigma(k)) \beta_k^* \alpha_k^* - \frac{1}{2} T(k) \alpha_{-k}^* \alpha_k^* - \frac{1}{2} T^*(k) \beta_{-k}^* \beta_k^*] a_k^* a_{-k}^* + \text{h.c.} \} + \\ & + (\omega_k - \Sigma(k)) |\alpha_{-k}|^2 - (\frac{1}{2} T(k) \alpha_k^* \beta_k + \text{h.c.}) \}. \end{aligned}$$

This expression is diagonal in a_k, a_k^* if the coefficient of $a_k^* a_{-k}^*$ is identically zero. The parameters α_k, β_k of the transformation which satisfy this condition turn out to be given by (1.15), together with a limitation on the phases im-

posed by

$$(2.7) \quad T(k) \alpha_{-k}^* \beta_k = |T(k) \alpha_{-k} \beta_k| .$$

Leaving out the additional zero-point energy we get finally

$$(2.8) \quad :\hat{H}: = \sum_k \sqrt{(\omega_k - \Sigma(k))^2 - |T(k)|^2} a_k^* a_k .$$

This Hamiltonian describes a system of free particles with energy $\hat{\omega}_k$ given by (2.1).

The Green function which describes the propagation of these quasi-phonons is

$$(2.9) \quad \tilde{G}(k, i\sigma) = \tilde{G}(-k, i\sigma) = \int_0^\beta d\tau \exp[-i\sigma\tau] \langle T \{a_k(\tau) a_k^*(0)\} \rangle .$$

With (2.8) one finds immediately that (2.9) is identical with (1.16) and hence with the function introduced in (1.14), whereas

$$\langle T \{a_{-k}^*(\tau) a_k^*(0)\} \rangle = \langle T \{a_k(\tau) a_{-k}(0)\} \rangle = 0 .$$

Accordingly the transformation (2.3) is equivalent in RPA to the relation

$$\langle T \{b_k(\tau) b_k^*(0)\} \rangle = |\alpha_k|^2 \langle T \{a_{-k}^*(\tau) a_{-k}(0)\} \rangle + |\beta_k|^2 \langle T \{a_k(\tau) a_k^*(0)\} \rangle ,$$

where on the left side the average is taken with $:\tilde{H}: (eq. (1.3))$ whereas on the right side it is with $:\hat{H}: (2.8)$. The Fourier-transformed relation reads with (2.9) and (1.2)

$$(2.10) \quad \tilde{g}(k, i\sigma) = |\alpha_k|^2 \tilde{G}(k, -i\sigma) + |\beta_k|^2 \tilde{G}(k, i\sigma) .$$

By use of (2.4') eq. (1.14) follows immediately from (2.10) and hence is equivalent in RPA to the inverse of the transformation (2.3)

$$(2.11) \quad a_k^* = \beta_k b_k^* - \alpha_{-k} b_{-k} .$$

3. - Discussion of the quasi-phonon.

In Sect. 1 and 2 we have shown how the phonon-number-nonconserving interactions modify the phonon propagators. The reason is that the latter will enter the structure equations for the collective-mode propagator and, in principle, we have to treat them both consistently in RPA.

We shall see now that this consistency is not essential for a qualitative analysis of the collective mode. The unique propagator (1.2) in the phonon number-

conserving approximation of part I will be sufficient for our purpose. It has the advantage of permitting the use of the same simple formalism as in part I, Sect. 11.

Indeed, the substitution of eq. (1.7') and eq. (D.8) of the Appendix into (1.5') and (1.6'), respectively, gives

$$(3.1) \quad \Sigma(k) = T(k) = T^*(k) = -\omega_k \cdot \frac{\lambda}{N} \sum_{\mathbf{k}'} \omega_{\mathbf{k}'} n_{\mathbf{k}'},$$

where n_k , is given by eq. (1.9).

Then the quasi-phonon energy (2.1) becomes

$$(3.2) \quad \hat{\omega}_k = \hat{\gamma} \cdot \omega_k,$$

where the renormalization factor $\hat{\gamma}$ is real and positive and is defined by

$$(3.3) \quad \hat{\gamma}^2 = 1 + 2 \frac{\lambda}{N} \sum_{\mathbf{k}'} \omega_{\mathbf{k}'} n_{\mathbf{k}'},$$

we get with (3.1)

$$(3.4) \quad \Sigma(k) = -\omega_k \cdot \frac{\hat{\gamma}^2 - 1}{2}.$$

Substitution of (1.9), (1.13), (3.1) and (3.4) into the expression for $\hat{\gamma}^2$ leads to the following equation for $\hat{\gamma}$:

$$\frac{1}{2} (\hat{\gamma}^2 - 1) = \lambda \beta^{-1} \cdot \frac{1}{N} \sum_{\mathbf{k}, \sigma} \omega_k \cdot \frac{\omega_k (1 + \frac{1}{2} (\hat{\gamma}^2 - 1)) - i\sigma}{\hat{\gamma}^2 \omega_k^2 + \sigma^2}.$$

With

$$\beta^{-1} \sum_{\sigma} (\hat{\gamma} \omega_k \pm i\sigma)^{-1} = (\exp [\beta \hat{\gamma} \omega_k] - 1)^{-1}$$

the equation becomes

$$(3.5) \quad \hat{\gamma} - 1 = \frac{\hat{\gamma}^2 + 1}{\hat{\gamma}(\hat{\gamma} + 1)} \cdot \frac{\lambda}{N} \sum_{\mathbf{k}} \frac{\omega_k}{\exp [\beta \hat{\gamma} \omega_k] - 1},$$

which is quite similar to eq. (I-3.12) for $\gamma \equiv \bar{\omega}_k / \omega_k$:

$$(3.6) \quad \gamma - 1 = \frac{\lambda}{N} \sum_{\mathbf{k}} \frac{\omega_k}{\exp [\beta \gamma \omega_k] - 1}.$$

Even the numerical solution of (3.5) for fixed λ and β differs insignificantly from $\gamma - 1$, as may be seen by evaluating the first iterative solution

$$\hat{\gamma} - 1 \simeq \frac{\gamma^2 + 1}{\gamma(\gamma + 1)} \cdot \frac{\lambda}{N} \sum_{\mathbf{k}} \frac{\omega_k}{\exp [\beta \gamma \omega_k] - 1}.$$

In order to test the accuracy of this approximation, we substitute into this expression (3.6) and take the factor $(\gamma^2 + 1)/\gamma(\gamma + 1)$ for $\gamma = \frac{3}{2}$, which is the largest value acceptable for $T \ll T_D$ according to the conclusions of part I. Then

$$\hat{\gamma} - 1|_{\gamma=\frac{3}{2}} \simeq \frac{13}{15} (\gamma - 1) .$$

Since with decreasing temperature the factor $(\gamma^2 + 1)/\gamma(\gamma + 1)$ approaches 1, the solutions of (3.5) and (3.6) give indeed almost the same renormalization of ω_k . Thus, as far as their energy is concerned, the quasi-phonons do not differ qualitatively from the phonons described in part I.

There remains the question whether the propagator $\tilde{g}_1(k, i\sigma)$ (eq. (1.2')) may cause an essential change in the propagation of the collective mode.

The answer is negative; it is based on the following argument.

The description of the phonon system by the Hamiltonian (1.1) necessitates an extension of the structure eq. (I-11.12) for the correlation function $\tilde{C}_{k,k'}(q, i\nu)$ where in particular the vertex (1.8) will appear. Owing to the orientation of the external lines of this function

$$(3.7) \quad \tilde{C}_{k,k'}(q, i\nu) = \begin{array}{c} \xrightarrow{k} \quad \quad \quad \xrightarrow{k'-q} \\ \quad \quad \quad \bigcirc \quad c \quad \quad \quad \\ \xleftarrow{k+q} \quad \quad \quad \xleftarrow{k'} \end{array} ,$$

the solution can only contain the propagator $\tilde{g}_1(k, i\sigma)$ (1.2') as connected to the different interaction vertices, in particular in the form

$$(3.8) \quad \begin{array}{c} \xrightarrow{\quad} \quad \quad \quad \xrightarrow{p} \\ \xleftarrow{(q, \sigma)} \quad \tau \quad \quad \quad \xleftarrow{p+l} \\ \xleftarrow{q+l} \quad \quad \quad \end{array}$$

corresponding to the vertex (1.7).

But at all places where this combination can be inserted, it adds to the topologically equivalent term

$$(3.9) \quad \begin{array}{c} \xrightarrow{\quad} \quad \quad \quad \xrightarrow{p} \\ \xleftarrow{(-q, -\sigma)} \quad \nu^* \quad \quad \quad \xleftarrow{p+l} \\ \xleftarrow{q+l} \quad \quad \quad \end{array} ,$$

corresponding to the vertex (1.8) and the propagator $\tilde{g}(-k, -i\sigma)$ (1.2).

Combining eqs. (1.12) and (1.13) shows that the analytic continuations $\tilde{g}(k, z)$ and $\tilde{g}_1(k, z)$ have the same singularity $\hat{\omega}_k$ (2.1), so that the combinations (3.8) and (3.9) produce qualitatively equivalent dynamical effects.

Now both vertices (1.7) and (1.8) are of the same order in the coupling parameter λ , whereas $\tilde{g}_1(k, i\sigma)$ is one order smaller than $\tilde{g}(k, i\sigma)$ according eq. (1.12).

equation (1) (I-11.6) we call them generalized B.S. equations. The generalization is limited in that nonconservation of the phonon number introduces new four-point vertices and consequently the functions (4.2) and (4.3), but no phonon propagator in addition to

$$(4.7) \quad \begin{array}{c} (1) \\ \leftarrow \\ \leftarrow \\ \leftarrow \end{array} \begin{array}{c} (2) \\ \leftarrow \\ \leftarrow \\ \leftarrow \end{array} = \int_0^\beta d\tau_1 \exp[-i\sigma_1 \tau_1] \int_0^\beta d\tau_2 \exp[i\sigma_2 \tau_2] \langle T \{b_{k_1}(\tau_1) b_{k_2}^*(\tau_2)\} \rangle \simeq \\ \simeq \beta \delta_{\sigma_1, \sigma_2} \delta_{k_1, k_2} \tilde{g}(k_1, i\sigma_1),$$

where (I-3.9)

$$(4.7') \quad \tilde{g}(k_1, i\sigma_1) \simeq (\bar{\omega}_k + i\sigma)^{-1}$$

according to the argument discussed in the previous Section.

The lowest-order approximation for the vertices

$$(4.8) \quad \begin{array}{c} (1) \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \boxed{\Gamma} \begin{array}{c} \rightarrow (2) \\ \rightarrow \\ \rightarrow \end{array} \begin{array}{c} (1') \leftarrow \\ \leftarrow \\ \leftarrow \end{array} \begin{array}{c} (2') \leftarrow \\ \leftarrow \\ \leftarrow \end{array} \simeq -\frac{\beta}{3!} \tau_{(-k'_1, -k_2)(k_1, k'_2)} \cdot \delta_{k'_1 - k_1, k'_2 - k_2} \cdot \delta_{\sigma'_1 - \sigma_1, \sigma'_2 - \sigma_2},$$

$$(4.9) \quad \begin{array}{c} (1) \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \boxed{\Gamma_1} \begin{array}{c} \leftarrow (-2) \\ \leftarrow \\ \leftarrow \end{array} \begin{array}{c} (1') \leftarrow \\ \leftarrow \\ \leftarrow \end{array} \begin{array}{c} (2') \leftarrow \\ \leftarrow \\ \leftarrow \end{array} \simeq -\frac{\beta}{4} v_{-k'_1(-k_2, k_1, k'_2)} \cdot \delta_{k'_1 - k_1, k'_2 - k_2} \cdot \delta_{\sigma'_1 - \sigma_1, \sigma'_2 - \sigma_2},$$

$$(4.10) \quad \begin{array}{c} (1) \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \boxed{\Gamma_2} \begin{array}{c} \leftarrow (-2) \\ \leftarrow \\ \leftarrow \end{array} \begin{array}{c} (-1') \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \begin{array}{c} (2') \leftarrow \\ \leftarrow \\ \leftarrow \end{array} \simeq -\beta \mu_{(-k'_1, -k_2, k_1, k'_2)} \cdot \delta_{k'_1 - k_1, k'_2 - k_2} \cdot \delta_{\sigma'_1 - \sigma_1, \sigma'_2 - \sigma_2}$$

gives the RPA.

For more simplicity we denote the set of variables of the functions like $\tilde{K}$ by

$$\left(\begin{array}{cc} k, i\sigma; & k', i\sigma' \\ k+q, i\sigma+iv; & k'-q, i(\sigma'-\nu') \end{array} \right) \equiv S$$

and mean by S'' the same set with (k, σ) replaced by (k'', σ'') . With use of (4.8) to (4.10) the system of equations (4.4) to (4.6) reduces to

$$(4.11) \quad \tilde{K}(S) \simeq \beta^2 \tilde{g}(k, i\sigma) \tilde{g}(k+q, i\sigma+iv) \cdot$$

$$\cdot \left\{ \delta_{\nu, \nu'} \delta_{\sigma', \sigma+\nu} \delta_{k', k+q} - \beta^{-3} \sum_{k'' \sigma''} \left(\frac{1}{3!} \tau_{(-k-q, -k'')(k, k''+q)} \cdot \tilde{K}(S'') + \right. \right. \\ \left. \left. + \frac{1}{4} v_{-k-q(-k'', k, k''+q)} \cdot \tilde{K}'(S'') + \frac{1}{4} v_{-k(k+q, k'', -k''-q)} \tilde{K}''(S'') \right) \right\},$$

(1) C. P. ENZ: in *Mathematical Methods in Solid State and Superfluid Theory*, Scottish Universities' Summer School, St. Andrews, 1967, edited by R. C. CLARK and G. H. DERRICK (Edinburgh, 1969), p. 339.

$$(4.12) \quad \tilde{K}'(S) \simeq -\beta^{-1} \tilde{g}(-k, -i\sigma) \tilde{g}(k+q, i\sigma + i\nu) \sum_{k''\sigma''} \left(\frac{1}{3!} \tau_{(-k-q, k)(k''+q, -k'')} \tilde{K}'(S'') + \right. \\ \left. + \frac{1}{4} \nu_{-k''-q(k+q, -k, k'')} \tilde{K}(S'') + \mu_{(k+q, -k''-q, -k, k'')} \tilde{K}'(S'') \right),$$

$$(4.13) \quad \tilde{K}''(S) \simeq -\beta^{-1} \tilde{g}(k, i\sigma) \tilde{g}(-k-q, -i\sigma - i\nu) \sum_{k''\sigma''} \left(\frac{1}{3!} \tau_{(k''+q, -k'')(-k-q, k)} \tilde{K}''(S'') + \right. \\ \left. + \frac{1}{4} \nu_{-k''(k, -k-q, k''+q)} \tilde{K}(S'') + \mu_{(k, -k-q, -k'', k''+q)} \tilde{K}'(S'') \right).$$

Starting from these equations we shall be able to calculate the propagator of the collective mode (I-11.1)

$$(4.14) \quad \mathbf{G}(q, \tau) \equiv \langle T\{c_q(\tau) c_q^*(0)\} \rangle$$

in RPA. But now, according to the Hamiltonian (1.1), the definitions (1.3) and (1.3') with $:\tilde{H}:$ are used for the average and for the imaginary time dependence instead of those with $\bar{H}$ (I-2.1).

5. - Collective-mode propagator.

Keeping in mind the modified meaning of the notation, we can again use the relation (I-11.3)

$$(5.1) \quad \mathbf{G}(q, \tau) = \sum_{kk'} \alpha_{k+q, k} \alpha_{k', k'-q}^* C_{k, k'}(q, \tau)$$

with the correlation-function ⁽²⁾ (I-11.2)

$$(5.2) \quad C_{k, k'}(q, \tau) \equiv \langle T\{\delta n_k(-q, \tau) \delta n_{k'}(q, 0)\} \rangle,$$

where $n_k(q)$ is given by (1.11).

Then the relation (I-11.5) also holds:

$$(5.3) \quad \tilde{C}_{k, k'}(q, i\nu) = \int_0^\beta d\tau \exp[-i\nu\tau] C_{k, k'}(q, \tau) = \beta^{-3} \sum_{\sigma, \sigma', \nu'} \tilde{K}(S).$$

⁽²⁾ C. P. ENZ: in *Theory of Condensed Matter, International Centre for Theoretical Physics, Trieste, 1967, IAEA* (Vienna, 1968), p. 762.

The sum of eq. (4.11) over σ, σ' and ν' multiplied by β^{-3} leads to the following equation for the correlation function (5.3) after analytic continuation $i\nu \rightarrow z$:

$$(5.4) \quad \tilde{C}_{k,k'}(q, z) = \tilde{L}_k(q, z) \left\{ \delta_{k', k+q} - \frac{1}{3!} \sum_{k''} \tau_{(-k-q, -k'') (k, k''+q)} \tilde{C}_{k'', k'}(q, z) - \right. \\ \left. - \frac{1}{4} \sum_{k''} (\nu_{-k-q(-k'', k, k''+q)} \tilde{C}'_{k'', k'}(q, z) + \nu_{-k(k+q, k'', -k''-q)}^* \tilde{C}''_{k'', k'}(q, z)) \right\},$$

where we have introduced the « Lindhard function » (I-11.10)

$$(5.5) \quad \tilde{L}_k(q, z) \equiv \beta^{-1} \sum_{\sigma} \tilde{g}(k, i\sigma) \tilde{g}(k+q, i\sigma+z)$$

and two new correlation functions

$$(5.6) \quad \tilde{C}'_{k,k'}(q, i\nu) \equiv \beta^{-3} \sum_{\sigma, \sigma', \nu'} \tilde{K}'(S),$$

$$(5.7) \quad \tilde{C}''_{k,k'}(q, i\nu) \equiv \beta^{-3} \sum_{\sigma, \sigma', \nu'} \tilde{K}''(S).$$

In the same way we obtain from (4.12)

$$(5.8) \quad \tilde{C}'_{k,k'}(q, z) = -\tilde{L}'_k(q, z) \sum_{k''} \left(\frac{1}{3!} \tau_{(-k-q, k'') (k''+q, -k'')} \tilde{C}_{k'', k'}(q, z) + \right. \\ \left. + \frac{1}{4} \nu_{-k''-q(k+q, -k'', k'')}^* \tilde{C}_{k'', k'}(q, z) + \mu_{(k+q, -k''-q, -k'', k'')}^* \tilde{C}''_{k'', k'}(q, z) \right)$$

and from (4.13)

$$(5.9) \quad \tilde{C}''_{k,k'}(q, z) = -\tilde{L}'_{k+q}(-q, -z) \sum_{k''} \left(\frac{1}{3!} \tau_{(k''+q, -k'') (-k-q, k)} \tilde{C}''_{k'', k'}(q, z) + \right. \\ \left. + \frac{1}{4} \nu_{-k''(k, -k-q, k''+q)} \tilde{C}_{k'', k'}(q, z) + \mu_{(k, -k-q, -k'', k''+q)} \tilde{C}'_{k'', k'}(q, z) \right).$$

Let us call the function introduced here

$$(5.10) \quad \tilde{L}'_k(q, z) \equiv \beta^{-1} \sum_{\sigma} \tilde{g}(-k, -i\sigma) \tilde{g}(k+q, i\sigma+z)$$

the « associated Lindhard function ».

From the Appendix (eqs. (D.7)-(D.9)) and from (I-2.8) we know that the vertex functions $\tau_{(\dots)(\dots)}, \nu_{\dots(\dots)}$ and $\mu_{(\dots)}$ factorize in the limit of long wave-

length $|q| \ll \pi/a$. This may be noted graphically in the form

$$(5.11) \quad -\frac{1}{3!} \tau_{(-k-q, -k'')(k, k''+q)} \simeq \begin{array}{c} k \\ \text{---} \text{---} \text{---} \end{array} \text{---} \begin{array}{c} k'' \\ \text{---} \text{---} \text{---} \end{array} \\ k+q \quad k''+q,$$

$$(5.11') \quad -\frac{1}{3!} \tau_{(-k-q, k')(k'', -k'')} \simeq \begin{array}{c} -k \\ \text{---} \text{---} \text{---} \end{array} \text{---} \begin{array}{c} -k'' \\ \text{---} \text{---} \text{---} \end{array} - \begin{array}{c} k \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} -k'' \\ \text{---} \text{---} \text{---} \end{array} \\ k+q \quad k''+q \quad k+q \quad k''+q,$$

$$(5.11'') \quad -\frac{1}{4} \tau_{(-k-q, -k'), k, k''+q} \simeq \begin{array}{c} k \\ \text{---} \text{---} \text{---} \end{array} \text{---} \begin{array}{c} -k'' \\ \text{---} \text{---} \text{---} \end{array} \\ k+q \quad k''+q,$$

$$(5.11''') \quad -\mu_{(k, -k-q, -k'', k''+q)} \simeq \begin{array}{c} k \\ \text{---} \text{---} \text{---} \end{array} \text{---} \begin{array}{c} -k'' \\ \text{---} \text{---} \text{---} \end{array} + \begin{array}{c} k \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} -k'' \\ \text{---} \text{---} \text{---} \end{array} \\ -k-q \quad k''+q \quad -k-q \quad k''+q,$$

where

$$(5.12) \quad \begin{array}{c} \pm k \\ \text{---} \text{---} \text{---} \end{array} = \begin{array}{c} \pm k \\ \text{---} \text{---} \text{---} \end{array} = i \left(\frac{\lambda}{N} \cdot \omega_k \omega_{k+q} \right)^{\frac{1}{2}}, \\ \pm(k+q)$$

$$(5.12') \quad \begin{array}{c} \pm k \\ \text{---} \text{---} \text{---} \end{array} = \begin{array}{c} \pm k \\ \text{---} \text{---} \text{---} \end{array} = i \frac{\lambda_3 \omega_0}{2(N\lambda_2^3)^{\frac{1}{2}}} \mathbf{P} \left(\frac{\omega_{k+q}}{\omega_k} \right)^{\frac{1}{2}} \\ \pm(k+q)$$

and $\mathbf{P}$ means the principal value in the sense

$$\frac{1}{x \pm i\varepsilon} = \frac{\mathbf{P}}{x} \mp i\pi\delta(x).$$

Then the eqs. (5.4), (5.8) and (5.9) read

$$(5.13) \quad \begin{array}{c} k \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k'-q \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k' \\ \text{---} \text{---} \text{---} \end{array} = \delta_{\mu', \mu+q} \cdot \begin{array}{c} k \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k+q \\ \text{---} \text{---} \text{---} \end{array} + \begin{array}{c} k \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k+q \\ \text{---} \text{---} \text{---} \end{array} \\ \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k'' \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k'-q \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k' \\ \text{---} \text{---} \text{---} \end{array} + \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} -k'' \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k'-q \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k' \\ \text{---} \text{---} \text{---} \end{array} + \left\{ \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k'' \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k'-q \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k' \\ \text{---} \text{---} \text{---} \end{array} + \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} -k'' \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k'-q \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k' \\ \text{---} \text{---} \text{---} \end{array} + \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k'' \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k'-q \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} k' \\ \text{---} \text{---} \text{---} \end{array} \right\},$$

$$\begin{aligned}
 (5.14) \quad & \begin{array}{c} \text{Diagram 1: Circle } C' \text{ with incoming } -k, \text{ outgoing } k'-q, \text{ and } k+q, k' \end{array} = \begin{array}{c} \text{Diagram 2: Circle } L' \text{ with incoming } -k, \text{ outgoing } -k, \text{ and } k+q, k+q \end{array} \left\{ \begin{array}{c} \text{Diagram 3: Circle } C' \text{ with incoming } -k'', \text{ outgoing } k'-q, \text{ and } k''+q, k' \\ \text{Diagram 4: Circle } C \text{ with incoming } k'', \text{ outgoing } k'-q, \text{ and } k''+q, k' \\ \text{Diagram 5: Circle } C'' \text{ with incoming } k'', \text{ outgoing } k'-q, \text{ and } -k''-q, k' \end{array} \right\} + \\
 & + \begin{array}{c} \text{Diagram 6: Circle } L' \text{ with incoming } -k, \text{ outgoing } k, \text{ and } k+q, k+q \end{array} \left\{ \begin{array}{c} \text{Diagram 7: Circle } C'' \text{ with incoming } k'', \text{ outgoing } k'-q, \text{ and } -k''-q, k' \\ \text{Diagram 8: Circle } C' \text{ with incoming } k'', \text{ outgoing } k'-q, \text{ and } k''+q, k' \end{array} \right\} + \\
 & + \begin{array}{c} \text{Diagram 9: Circle } L' \text{ with incoming } -k, \text{ outgoing } k, \text{ and } k+q, k+q \end{array} \left\{ \begin{array}{c} \text{Diagram 10: Circle } C'' \text{ with incoming } k'', \text{ outgoing } k'-q, \text{ and } -k''-q, k' \\ \text{Diagram 11: Circle } C' \text{ with incoming } -k'', \text{ outgoing } k'-q, \text{ and } k''+q, k' \end{array} \right\},
 \end{aligned}$$

$$\begin{aligned}
 (5.15) \quad & \begin{array}{c} \text{Diagram 12: Circle } C'' \text{ with incoming } k, \text{ outgoing } k'-q, \text{ and } k-q, k' \end{array} = \begin{array}{c} \text{Diagram 13: Circle } L'' \text{ with incoming } k, \text{ outgoing } k, \text{ and } -k-q, -k-q \end{array} \left\{ \begin{array}{c} \text{Diagram 14: Circle } C'' \text{ with incoming } k'', \text{ outgoing } k'-q, \text{ and } -k''-q, k' \\ \text{Diagram 15: Circle } C \text{ with incoming } k'', \text{ outgoing } k'-q, \text{ and } k''+q, k' \\ \text{Diagram 16: Circle } C' \text{ with incoming } -k'', \text{ outgoing } k'-q, \text{ and } k''+q, k' \end{array} \right\} + \\
 & + \begin{array}{c} \text{Diagram 17: Circle } L'' \text{ with incoming } k, \text{ outgoing } k, \text{ and } -k-q, -k-q \end{array} \left\{ \begin{array}{c} \text{Diagram 18: Circle } C' \text{ with incoming } k'', \text{ outgoing } k'-q, \text{ and } -k''-q, k' \\ \text{Diagram 19: Circle } C'' \text{ with incoming } k'', \text{ outgoing } k'-q, \text{ and } k''+q, k' \end{array} \right\},
 \end{aligned}$$

where we have introduced for convenience

$$(5.10') \quad \tilde{L}_k''(q, z) \equiv \tilde{L}_{k+q}'(-q, -z).$$

With the definition (I-11.13)

$$(5.16) \quad \triangleleft \begin{array}{c} k \\ k+q \end{array} = \alpha_{k+q, k} ; \quad \begin{array}{c} k-q \\ k \end{array} \triangleright = \alpha_{k, k-q} \dots$$

eq. (5.1) reads after Fourier transformation according to (5.3)

$$(5.17) \quad \tilde{\mathbf{G}}(q, z) = \triangleleft \begin{array}{c} \text{Diagram 20: Circle } C \end{array} \triangleright.$$

But now multiplication of (5.13) by the two quantities of (5.16) and summation over k and k' leads to the equation (instead of (I-11.14))

$$\begin{aligned}
 (5.18) \quad & \triangleleft \begin{array}{c} \text{Diagram 21: Circle } C \end{array} \triangleright - \triangleleft \begin{array}{c} \text{Diagram 22: Circle } L \end{array} \triangleright + \triangleleft \begin{array}{c} \text{Diagram 23: Circle } L \end{array} \triangleright \left\{ \begin{array}{c} \text{Diagram 24: Circle } C \end{array} \triangleright + \right. \\
 & \left. + \begin{array}{c} \text{Diagram 25: Circle } C' \end{array} \triangleright + \begin{array}{c} \text{Diagram 26: Circle } C'' \end{array} \triangleright \dots \right.
 \end{aligned}$$

This introduces three additional functions,

$$(5.19) \quad \tilde{\mathbf{F}}(q, z) = i \sqrt{\frac{\lambda}{N}} \sum_{k, k'} \sqrt{\omega_k \omega_{k+q}} \tilde{C}_{k, k'}(q, z) \alpha_{k', k'-q}^* = \text{Diagram } C, \quad ,$$

$$(5.19') \quad \tilde{\mathbf{F}}'(q, z) = i \sqrt{\frac{\lambda}{N}} \sum_{k, k'} \sqrt{\omega_k \omega_{k+q}} \tilde{C}'_{k, k'}(q, z) \alpha_{k', k'-q}^* = \text{Diagram } C', \quad ,$$

$$(5.19'') \quad \tilde{\mathbf{F}}''(q, z) = i \sqrt{\frac{\lambda}{N}} \sum_{k, k'} \sqrt{\omega_k \omega_{k+q}} \tilde{C}''_{k, k'}(q, z) \alpha_{k', k'-q}^* = \text{Diagram } C'', \quad ,$$

for which the equations

$$(5.20) \quad \text{Diagram } C = \text{Diagram } L + \text{Diagram } L \left\{ \text{Diagram } C + \text{Diagram } C' + \text{Diagram } C'' \right\},$$

$$(5.20') \quad \text{Diagram } C' = \text{Diagram } L' \left\{ \text{Diagram } C'' - \text{Diagram } C' \right\} + \text{Diagram } L' \left\{ \text{Diagram } C + \text{Diagram } C' + \text{Diagram } C'' \right\},$$

$$(5.20'') \quad \text{Diagram } C'' = \text{Diagram } L'' \left\{ \text{Diagram } C' - \text{Diagram } C'' \right\} + \text{Diagram } L'' \left\{ \text{Diagram } C + \text{Diagram } C' + \text{Diagram } C'' \right\},$$

follow from (5.13), (5.14) and (5.15).

From the last two of these equations we get similarly

$$(5.21) \quad \text{Diagram } C' = \text{Diagram } L' \left\{ \text{Diagram } C'' - \text{Diagram } C' \right\} + \text{Diagram } L' \left\{ \text{Diagram } C + \text{Diagram } C' + \text{Diagram } C'' \right\},$$

$$(5.21') \quad \begin{array}{c} \text{Diagram with circle } C'' \text{ and left half-shaded} \\ \text{Diagram with circle } L'' \text{ and both halves shaded} \end{array} = \begin{array}{c} \text{Diagram with circle } C' \text{ and left half-shaded} \\ \text{Diagram with circle } C'' \text{ and left half-shaded} \end{array} + \\ + \begin{array}{c} \text{Diagram with circle } L'' \text{ and left half-shaded} \\ \text{Diagram with circle } C \text{ and left half-shaded} \\ \text{Diagram with circle } C' \text{ and left half-shaded} \\ \text{Diagram with circle } C'' \text{ and left half-shaded} \end{array},$$

for the last two functions needed,

$$(5.22) \quad \tilde{\mathbf{E}}'(q, z) = \frac{i\lambda_3\omega_0}{2} \sqrt{\frac{1}{N\lambda_2^3}} \sum_{k,k'} \sqrt{\frac{\omega_{k+q}}{\omega_k}} \tilde{C}_{k,k'}'(q, z) \cdot \alpha_{k',k'-q}^* = \text{Diagram with circle } C' \text{ and left half-shaded},$$

$$(5.22') \quad \tilde{\mathbf{E}}''(q, z) = \frac{i\lambda_3\omega_0}{2} \sqrt{\frac{1}{N\lambda_2^3}} \sum_{k,k'} \sqrt{\frac{\omega_{k+q}}{\omega_k}} \tilde{C}_{k,k'}''(q, z) \cdot \alpha_{k',k'-q}^* = \text{Diagram with circle } C'' \text{ and left half-shaded}.$$

Onwards from eq. (5.20) we have dropped the arrows in the symbols for simplicity because through eqs. (5.13) to (5.15) and (5.10') they are fixed uniquely by indicating the type of function. Thus we have a system of six linear inhomogeneous equations for the six unknown functions $\tilde{\mathbf{G}}, \tilde{\mathbf{F}}, \tilde{\mathbf{F}}', \tilde{\mathbf{F}}'', \tilde{\mathbf{E}}'$, and $\tilde{\mathbf{E}}''$. The only one we are interested in is the collective-mode propagator $\tilde{\mathbf{G}}(q, z)$. Solving the system for the latter we get

$$(5.23) \quad \begin{array}{c} \text{Diagram with circle } C \text{ and both halves shaded} \\ \text{Diagram with circle } L \text{ and both halves shaded} \end{array} = \begin{array}{c} \text{Diagram with circle } L \text{ and both halves shaded} \\ \text{Diagram with circle } L \text{ and both halves shaded} \end{array} \cdot \\ \cdot \left[1 - \begin{array}{c} \text{Diagram with circle } L \text{ and both halves shaded} \\ \text{Diagram with circle } L' \text{ and both halves shaded} \end{array} + \begin{array}{c} \text{Diagram with circle } L'' \text{ and both halves shaded} \end{array} + \right. \\ + \left[\begin{array}{c} \text{Diagram with circle } L' \text{ and left half-shaded} \\ \text{Diagram with circle } L'' \text{ and left half-shaded} \end{array} \cdot \begin{array}{c} \text{Diagram with circle } L' \text{ and left half-shaded} \\ \text{Diagram with circle } L'' \text{ and left half-shaded} \end{array} \cdot \right. \\ \left. \cdot \left(1 + \begin{array}{c} \text{Diagram with circle } L' \text{ and left half-shaded} \\ \text{Diagram with circle } L'' \text{ and left half-shaded} \end{array} \right) \right],$$

which can be rearranged as

$$(5.23') \quad \begin{array}{c} \text{Diagram with circle } C \text{ and both halves shaded} \\ \text{Diagram with circle } L \text{ and both halves shaded} \end{array} = \begin{array}{c} \text{Diagram with circle } L \text{ and both halves shaded} \\ \text{Diagram with circle } L \text{ and both halves shaded} \end{array} + \\ + \frac{\begin{array}{c} \text{Diagram with circle } L \text{ and both halves shaded} \\ \text{Diagram with circle } L \text{ and both halves shaded} \end{array}}{\begin{array}{c} \text{Diagram with circle } L \text{ and both halves shaded} \\ \text{Diagram with circle } L \text{ and both halves shaded} \end{array}} + \frac{\begin{array}{c} \text{Diagram with circle } L \text{ and both halves shaded} \\ \text{Diagram with circle } L \text{ and both halves shaded} \end{array}}{\begin{array}{c} \text{Diagram with circle } L \text{ and both halves shaded} \\ \text{Diagram with circle } L \text{ and both halves shaded} \end{array}} + \Sigma$$

where

$$(5.24) \quad \Sigma(q, z) =$$

$$= \textcircled{\Sigma} \equiv \left\{ - \left(\textcircled{L'} + \textcircled{L''} \right) + \right. \\ \left. + \frac{\left(\textcircled{L'} - \textcircled{L''} \right) \cdot \left(\textcircled{L'} - \textcircled{L''} \right)}{1 + \textcircled{L'} + \textcircled{L''}} \right\} \cdot \left\{ \textcircled{L} \left(1 - \textcircled{L} \right) + \textcircled{L} \right\}^{-1}.$$

In the denominator of (5.23') we recognize the propagator (I-11.17) calculated with $\bar{H}$ (I-2.1) which describes the undamped collective mode. Using the result (I-11.22) we denote it here

$$(2.25) \quad \tilde{\mathbf{G}}^0(q, z) = (\Omega_q + z)^{-1},$$

where Ω_q is the solution of the eigenvalue equation (I-4.6).

According to eqs. (11.17), (11.19), (11.20) and (11.21) of I we have

$$(5.26) \quad \left\{ \begin{aligned} \textcircled{L} &= (z + \Omega_q)^{-1} \cdot (1 - \zeta_q(z)), \\ \textcircled{L} \textcircled{L} &= (z + \Omega_q)^{-1} \cdot (1 - F_q(z)) \cdot \zeta_q(z), \\ \textcircled{L} (1 - \textcircled{L}) + \textcircled{L} &= \frac{1 - F_q(z)}{z + \Omega_q}, \end{aligned} \right.$$

where

$$\zeta_q(z) = \frac{F_q(z) - 1}{z + \Omega_q} \cdot \frac{N}{\lambda} \cdot |N_q|^2,$$

according to (I-4.7) takes the form

$$(5.27) \quad \zeta_q(z) = \frac{1 - F_q(z)}{z + \Omega_q} \cdot \left(\frac{dF_q(z)}{dz} \Big|_{z=\Omega_q} \right)^{-1}.$$

$F_q(z)$ is the «dynamical function» defined in (I.4.6')

$$(5.28) \quad F_q(z) \equiv \frac{\lambda}{N} \sum_k \frac{\omega_k \omega_{k-q}}{z - (\bar{\omega}_k - \bar{\omega}_{k-q})} \cdot (\bar{n}_{k-q} - \bar{n}_k),$$

where $\bar{n}_k$ and $\bar{\omega}_k$ are given by (I.3.10), (I.3.11).

Then with (5.17) eq. (5.23') reads

$$(5.29) \quad \tilde{\mathbf{G}}(q, z) = \frac{1 - \zeta_q(z)}{z + \Omega_q} + \frac{\zeta_q(z)}{z + \Omega_q + \Sigma(q, z)}.$$

Thus $\Sigma(q, z)$ is the self-energy of the collective mode due to the phonon-number-nonconserving interactions in $:\tilde{\mathcal{H}}:$ (I.1), whereas $\zeta_q(z)$ appears as a generalization of the wave-function renormalization factor z_q ⁽²⁾ in eq. (I-11.23), the regular part being here $(1 - \zeta_q(z)) \cdot (z + \Omega_q)^{-1}$.

6. - The self-energy $\Sigma(q, z)$.

The formula for $\Sigma(q, z)$ follows from the meaning of the different symbols which enter eq. (5.24).

The denominator is already known from eq. (5.26). Then we have with (5.12)

$$\left(\text{Diagram: circle with } L' \text{ inside, two semi-circles on the left and right} \right) = -\frac{\lambda}{N} \sum_k \omega_k \omega_{k+q} \tilde{L}'_k(q, z),$$

which becomes after substitution of (5.10) and (4.7')

$$(6.1) \quad \left(\text{Diagram: circle with } L' \text{ inside, two semi-circles on the left and right} \right) = -\frac{\lambda}{N} \sum_k \frac{\omega_k \omega_{k+q} (1 + \bar{n}_k + \bar{n}_{k+q})}{\bar{\omega}_k + \bar{\omega}_{k+q} + z} = \mathcal{L}_1(q, z).$$

Similarly (5.10') leads to

$$(6.1') \quad \left(\text{Diagram: circle with } L'' \text{ inside, two semi-circles on the left and right} \right) = -\frac{\lambda}{N} \sum_k \omega_k \omega_{k+q} \tilde{L}''_k(q, z) = \mathcal{L}_1(q, -z).$$

The same procedure with (5.12) and (5.12') gives

$$(6.2) \quad \left(\text{Diagram: circle with } L' \text{ inside, semi-circle on the left, shaded semi-circle on the right} \right) = -\left(\frac{\lambda}{\lambda_2^3} \right)^{\frac{1}{2}} \frac{\lambda_3 \omega_0}{2} \cdot \frac{\mathbf{P}}{N} \sum_k \frac{\omega_{k+q} (1 + \bar{n}_k + \bar{n}_{k+q})}{\bar{\omega}_k + \bar{\omega}_{k+q} + z} \equiv \mathcal{L}_2(q, z),$$

$$(6.2') \quad \left(\text{Diagram: circle with } L'' \text{ inside, semi-circle on the left, shaded semi-circle on the right} \right) = -\left(\frac{\lambda}{\lambda_2^3} \right)^{\frac{1}{2}} \frac{\lambda_3 \omega_0}{2} \cdot \frac{\mathbf{P}}{N} \sum_k \omega_{k+q} \tilde{L}''_k(q, z) = \mathcal{L}_2(q, -z),$$

$$(6.3) \quad \left(\text{Diagram: circle with } L' \text{ inside, shaded semi-circles on both left and right} \right) = -\frac{(\lambda_3 \omega_0)^3}{4 \lambda_2^3} \cdot \frac{\mathbf{P}}{N} \sum_k \frac{\omega_{k+q}}{\omega_k} \cdot \frac{1 + \bar{n}_k + \bar{n}_{k+q}}{\bar{\omega}_k + \bar{\omega}_{k+q} + z} \equiv \mathcal{L}_3(q, z),$$

$$(6.3') \quad \left(\text{Diagram: circle with } L'' \text{ inside, shaded semi-circles on both left and right} \right) = -\frac{(\lambda_3 \omega_0)^2}{4 \lambda_2^3} \cdot \frac{\mathbf{P}}{N} \sum_k \frac{\omega_{k+q}}{\omega_k} \tilde{L}''_k(q, z) = \mathcal{L}_3(q, -z).$$

Substitution of these expressions with (5.26) into (5.24) gives

$$(6.4) \quad \Sigma(q, z) = \frac{z + \Omega_q}{F_q(z) - 1} (\mathcal{L}_1(q, z) + \mathcal{L}_1(q, -z)) + \\ + \frac{z + \Omega_q}{1 - F_q(z)} \cdot \frac{(\mathcal{L}_2(q, z) - \mathcal{L}_2(q, -z))(\mathcal{L}_3(q, z) - \mathcal{L}_3(q, -z))}{1 + \mathcal{L}_3(q, z) + \mathcal{L}_3(q, -z)}.$$

From this quantity we obtain the line width of the spectral function which belongs to the propagator (5.29) of the collective mode. Following ref. (3), (referring in particular to eqs. (4-19) and (4-21)) the line shift is given by

$$(6.5) \quad \Delta_q(\omega) = \text{Re } \Sigma(q, \omega \pm i\varepsilon)$$

and the line width by

$$(6.6) \quad \pm \Gamma_q(\omega) = -\text{Im } \Sigma(q, \omega \pm i\varepsilon),$$

where ω is a real energy.

The spectral function which belongs to the propagator (5.25) of the undamped collective mode is a δ -function peaked at $\omega = -\Omega_q$. In order to get the renormalization of the collective-mode energy Ω_q by phonon-number non-conservation, we have to evaluate $\Delta_q(\omega)$ and $\Gamma_q(\omega)$ at

$$\omega = -[\Omega_q + \Delta_q(\Omega_q + \Delta_q(\dots))].$$

Assuming $|\Delta_q| \ll |\Omega_q|$, which actually will turn out to be true, we shall calculate in first approximation (6.5) and (6.6) for $\omega = -\Omega_q$.

Now according (6.2), (6.2'), (6.3) and (6.3'), the second term of (6.4) is

$$\frac{(z + \Omega_q) \cdot \frac{1}{2} z^2 \cdot \left(\frac{\lambda}{\lambda_2^3}\right)^{\frac{1}{2}} \left(\frac{\lambda_3 \omega_0}{\lambda_2}\right)^3 \frac{\mathbf{P}}{N} \sum_k \frac{\omega_{k+q} (1 + \bar{n}_k + \bar{n}_{k+q})}{(\bar{\omega}_k + \bar{\omega}_{k+q})^2 - z^2} \cdot \frac{\mathbf{P}}{N} \sum_{k'} \frac{\omega_{k'+q} \cdot (1 + \bar{n}_{k'} + \bar{n}_{k'+q})}{(\bar{\omega}_{k'} + \bar{\omega}_{k'+q})^2 - z^2}}{(1 - F_q(z)) \left(1 - \frac{(\lambda_3 \omega_0)^2}{2 \lambda_2^3} \cdot \frac{\mathbf{P}}{N} \sum_k \frac{\omega_{k+q} \cdot (\bar{\omega}_k + \bar{\omega}_{k+q}) (1 + \bar{n}_k + \bar{n}_{k+q})}{(\bar{\omega}_k + \bar{\omega}_{k+q})^2 - z^2}\right)},$$

whereas the first term of (6.4) is with (6.1), (6.1')

$$(6.7) \quad 2 \frac{z + \Omega_q}{1 - F_q(z)} \cdot \frac{\lambda}{N} \sum_k \frac{\omega_k \omega_{k+q} (\bar{\omega}_k + \bar{\omega}_{k+q}) (1 + \bar{n}_k + \bar{n}_{k+q})}{(\bar{\omega}_k + \bar{\omega}_{k+q})^2 - z^2} \equiv \Sigma^{(1)}(q, z).$$

(3) L. P. KADANOFF and G. BAYM: *Quantum Statistical Mechanics* (New York, 1962).

The combination of coupling parameters $(\lambda/\lambda_2)^{\frac{1}{2}} \cdot (\lambda_3/\lambda_2)^3$ is of the same order as λ^2 , so that the second term of (6.4) is negligible compared to (6.7) for weak coupling $\lambda\omega_0 \ll 1$ which we shall assume. Moreover, the factor z^2 in front of the former, absent in (6.7) makes that in orders of $|q| \ll \pi/a$ the dominant contribution to $\Sigma(q, -\Omega_q \pm i\varepsilon)$ is given by (6.7).

Thus, in the limit of long wavelength we have to the lowest order in $|q|$ and $\lambda\omega_0$:

$$(6.8) \quad \Sigma(q, -\Omega_q \pm i\varepsilon) \simeq \Sigma^{(1)}(q, -\Omega_q \pm i\varepsilon).$$

7. - Line shift and line width for $T \ll T_D$.

Now that we have established that the phonon-number-nonconserving interactions which we neglected in Part I lead to a self-energy for the collective mode, we have to verify whether the line shift and the line width are small compared to the energy $\Omega_q \simeq v_H \cdot |q|$ or not. If they are, the phonon-number-conserving approximation of I is justified.

We shall outline here the calculation for weak coupling $\lambda\omega_0 \ll 1$ and temperatures $T \ll T_D$ (*i.e.* $\beta\omega_0 \gg 1$). According to the discussion in the preceding Section and eqs. (6.5), (6.7) and (6.8), the shift of the line peaked at $-\Omega_q$, the pole of the unperturbed propagator (5.25), is equal to

$$\Delta_q(-\Omega_q) = - \left(\frac{dF_q(z)}{dz} \Big|_{z=-\Omega_q} \right)^{-1} \otimes \lambda \frac{P}{N} \sum_k \omega_k \omega_{k+q} (1 + \bar{n}_k + \bar{n}_{k+q}) \frac{2(\bar{\omega}_k + \bar{\omega}_{k+q})}{(\bar{\omega}_k + \bar{\omega}_{k+q})^2 - \Omega_q^2}.$$

With eqs. (I-4.7) and (I-3.11) we may write after replacing the summation variable k by $k - q/2$:

$$(7.1) \quad \Delta_q(-\Omega_q) = - |N_q|^2 \frac{P}{\gamma^2} \cdot \sum_{k=-\pi/a+|q/2|}^{\pi/a-|q/2|} \left\{ \bar{\omega}_{k-q/2} \bar{\omega}_{k+q/2} (1 + \bar{n}_{k-q/2} + \bar{n}_{k+q/2}) \otimes \frac{2(\bar{\omega}_{k-q/2} + \bar{\omega}_{k+q/2})}{(\bar{\omega}_{k-q/2} + \bar{\omega}_{k+q/2})^2 - \Omega_q^2} \right\}.$$

Obviously $\Delta_q(-\Omega_q)$ depends on the absolute value of q , so that we may assume $q > 0$ in what follows instead of writing $|q|$.

The sum in (7.1) splits up into two parts, due to the form of the phonon spectrum (I-5.5):

$$(7.2) \quad \bar{\omega}_k = \bar{\omega}_0 \left| \sin \frac{ak}{2} \right|,$$

$$(7.3) \quad \bar{\omega}_0 = \gamma\omega_0,$$

where the maximum energy (7.3) is related to the sound velocity by

$$(7.4) \quad v_{\mathbf{I}} = \frac{a\bar{\omega}_0}{2}$$

and a is the inter-atomic distance of the linear chain. Indeed, (7.2) implies

$$\text{for } |k| \leq q/2$$

$$(7.5) \quad \bar{\omega}_{k+q/2} + \bar{\omega}_{k-q/2} = 2 \cos \frac{ak}{2} \cdot \bar{\omega}_{q/2},$$

$$\text{for } |k| \geq q/2$$

$$(7.5') \quad \bar{\omega}_{k+q/2} + \bar{\omega}_{k-q/2} = 2 \cos \frac{aq}{4} \cdot \bar{\omega}_k.$$

With these expressions, it turns out that the zero of the denominator in (7.1) is, for the case (7.5),

$$(7.6) \quad \left(\frac{ak_0}{2} \right)^2 \simeq 2 - (v_{\mathbf{II}}/v_{\mathbf{I}}),$$

where use was made of $\Omega_a \simeq v_{\mathbf{II}} \cdot |q|$, according to Sect. 5 of I, and of eq. (7.4). For the case (7.5') the zero of the denominator in (7.1) is given by

$$(7.6') \quad k_0 \simeq (v_{\mathbf{II}}/v_{\mathbf{I}}) \cdot q/2.$$

Under the conditions assumed here the maximum of $v_{\mathbf{II}}/v_{\mathbf{I}}$ (see Part I) is about 1.005, whereas in the long-wavelength limit $q \ll \pi/a$ holds. Consequently (7.6) is incompatible with $|k| \leq q/2$ and the zero k_0 is given by (7.6'). With (7.2), (7.4), (7.5) and (7.5') eq. (7.1) can be written in the limit of an infinite chain, $N \rightarrow \infty$, as

$$(7.7) \quad \Delta_a(-v_{\mathbf{II}}|q|) \simeq -|N_a|^2 \cdot \left\{ \frac{2N}{\gamma^2} \left[\frac{a}{\pi} \int_0^{q/2} dk \left[\frac{-v_{\mathbf{I}}^2 \cdot (k - q/2)(k + q/2) \cdot v_{\mathbf{I}} \cdot q}{(v_{\mathbf{I}}q)^2 - (v_{\mathbf{II}}q)^2} \otimes \left(1 + \frac{1}{\beta v_{\mathbf{I}}(k + q/2)} - \frac{1}{\beta v_{\mathbf{I}}(k - q/2)} \right) \right] + \right. \right. \\ \left. \left. + \frac{a}{\pi} \mathbf{P} \int_{q/2}^{\pi/a - q/2} dk \frac{2\bar{\omega}_0^3 \sin^3 ak/2}{4\bar{\omega}_0^2 \sin^2 ak/2 - (v_{\mathbf{II}}q)^2} \cdot \left(1 + \frac{2}{\exp[\beta \bar{\omega}_0 \cdot \sin ak/2] - 1} \right) \right] \right\}.$$

The approximations made are based on the assumption of a very long wave length

$$(7.8) \quad \left| \beta \bar{\omega}_0 \cdot \frac{aq}{2} \right| = \beta v_{\mathbf{I}}q \ll 1,$$

where $\beta \equiv (k_B \cdot T)^{-1}$. This allows in particular the simple approximation in the first term for the phonon distribution (I-3.10). Let us write for the two contributions in (7.7)

$$(7.7') \quad A_q(-v_{\text{II}}|q|) \simeq -\frac{2N}{\gamma^2} |N_q|^2 \cdot (J_1 + J_2).$$

To lowest order in q , the first integral gives

$$(7.9) \quad J_1 \simeq \frac{v_{\text{I}} q}{\pi \alpha \beta \bar{\omega}_0},$$

where (I-6.1)

$$(7.10) \quad \alpha \equiv (v_{\text{II}}/v_{\text{I}})^2 - 1.$$

It is possible to evaluate the second integral by separation of the integration interval (see also Sect. 7 of Part I) and approximating the integrand as follows:

$$(7.11) \quad \text{i) } x \equiv \frac{ak}{2} \leq \frac{v_{\text{II}}}{v_{\text{I}}} \cdot \frac{aq}{2} \equiv \bar{x},$$

$\sin x \simeq x$, $(\exp[\beta \bar{\omega}_0 \sin x] - 1)^{-1} \simeq (\beta \bar{\omega}_0 \cdot x)^{-1}$. This interval $aq/4 \leq x \leq \bar{x}$ contains the singularity (7.6') of the integrand. The principal value of this integral to lowest order in $|q|$, the temperature T/T_D and the coupling parameter $\lambda \omega_0$ (implicit in $(v_{\text{II}}/v_{\text{I}}) - 1$) is found to be

$$(7.11') \quad J_2^{(i)} \simeq -\frac{\bar{\omega}_0}{2\pi} \cdot \frac{1}{\gamma} \cdot \frac{T}{T_D} \cdot \frac{v_{\text{II}}}{v_{\text{I}}} \cdot \frac{aq}{2} \left| \ln \left\{ \frac{v_{\text{II}}}{v_{\text{I}}} - 1 \right\} \right|.$$

ii) $x \geq \bar{x}$; ($\bar{x}$ defined by (7.11)).

The contribution of the phonon distribution $(\exp[\beta \bar{\omega}_0 \cdot \sin x] - 1)^{-1}$ within

$$J_2^{(ii)} = \frac{a^2}{\pi} \int_{(v_{\text{II}}/v_{\text{I}})(aq/2)}^{\pi/2} dx \frac{\bar{\omega}_0^3 \cdot \sin^3 x}{4v_{\text{I}}^2 \sin x - v_{\text{II}}^2 (aq/2)^2} \left(1 + \frac{2}{\exp[\beta \bar{\omega}_0 \sin x] - 1} \right)$$

has to be calculated separately using the variable $y = \beta \bar{\omega}_0 \cdot \sin x$ and leads to

$$(7.12) \quad \frac{a^2 \beta^{-2} \bar{\omega}_0}{2\pi v_{\text{I}}^2} \int_{\beta \bar{\omega}_0 (v_{\text{II}}/v_{\text{I}})(aq/2)}^{\beta \bar{\omega}_0} \frac{dy}{\sqrt{1 - (y/\beta \bar{\omega}_0)^2}} \cdot \frac{y^3 (\exp[y] - 1)^{-1}}{y^2 - \frac{1}{4} (\beta \bar{\omega}_0 (v_{\text{II}}/v_{\text{I}})(aq/2))^2},$$

whereas the other term can be transformed to a rational function of t by $\text{tg}(x/2) = t$ and integrated exactly.

In the contribution (7.12) the rapid decreasing of the Bose-function with increasing y allows us to neglect the q -dependence in the denominator, at least for a qualitative estimate, by setting $q = 0$.

The integration by parts leads to

$$\begin{aligned} \frac{a}{2\pi} \cdot \frac{1}{\beta^2 v_{\text{I}}} \left\{ (\beta \bar{\omega}_0)^2 \sqrt{1 - \left(\frac{v_{\text{II}}}{v_{\text{I}}} \cdot \frac{aq}{2} \right)^2} \cdot \frac{((v_{\text{II}}/v_{\text{I}})(aq/2))^2}{\exp[\beta \bar{\omega}_0 (v_{\text{II}}/v_{\text{I}})(aq/2)] - 1} + \right. \\ \left. + \int_{\beta \bar{\omega}_0 (v_{\text{II}}/v_{\text{I}})(aq/2)}^{\beta \bar{\omega}_0} dy \sqrt{1 - \left(\frac{y}{\beta \bar{\omega}_0} \right)^2} \left(\frac{2y}{\exp[y] - 1} + \frac{d}{dy} \frac{y^2}{\exp[y] - 1} \right) \right\}. \end{aligned}$$

This integral is evaluated in the same way as (I-7.8) neglecting the square root. The final result to lowest order in q and T/T_{D} is

$$(7.13) \quad J_2^{(ii)} \sim -\frac{\bar{\omega}_0}{\pi} \left(1 + \frac{1}{4} \left(\frac{v_{\text{II}}}{v_{\text{I}}} \cdot \frac{aq}{2} \right)^2 \cdot \log \left(\frac{v_{\text{II}}}{v_{\text{I}}} \cdot \frac{aq}{2} \right) \right).$$

Quantitatively, the logarithmic term could be neglected, but for qualitative information, it is of interest to point out other q -dependences than powers.

The sum of (7.9), (7.11) and (7.13) substituted into (7.7') together with (I-4.7) and (I-8.4) leads to

$$\begin{aligned} \Delta_q(-v_{\text{II}}|q|) \simeq -v_{\text{II}}q \frac{\alpha}{2(\alpha + 1)} \cdot \left(1 - \frac{8\lambda\omega_0}{3\pi\gamma^2 \sqrt{\alpha}\beta\omega_0} \cdot \frac{3}{(\sqrt{\alpha}\beta\omega_0\gamma)^3} \int_0^{\sqrt{\alpha}\gamma\beta\omega_0} \frac{y^3 dy}{\exp[y] - 1} \right)^{-1} \otimes \\ \otimes \frac{2\lambda\bar{\omega}_0}{\pi\gamma^2} \left(\frac{1}{\alpha\gamma} \cdot \frac{T}{T_{\text{D}}} \cdot \frac{v_{\text{I}}q}{\bar{\omega}_0} - 1 - \frac{1}{2\gamma} \cdot \frac{T}{T_{\text{D}}} \cdot \left(\frac{v_{\text{II}}}{v_{\text{I}}} \cdot \frac{aq}{2} \right) \log \left(\frac{v_{\text{II}}}{v_{\text{I}}} - 1 \right) - \frac{1}{4} \left(\frac{v_{\text{II}}}{v_{\text{I}}} \cdot \frac{aq}{2} \right)^2 \log \left(\frac{v_{\text{II}}}{v_{\text{I}}} \cdot \frac{aq}{2} \right) \right). \end{aligned}$$

According to (I-7.7) $\sqrt{\alpha}\gamma\beta\omega_0 < 2\pi$ and the series (I-6.5) generating the Bernoulli numbers can be used for

$$\frac{3}{(\sqrt{\alpha}\gamma\beta\omega_0)^3} \int_0^{\sqrt{\alpha}\gamma\beta\omega_0} \frac{y^3 dy}{\exp[y] - 1} = \sum_{n=0}^{\infty} \frac{3}{n+3} \cdot \frac{B_n}{n!} \cdot (\sqrt{\alpha}\gamma\beta\omega_0)^n.$$

To lowest order in q , $\lambda\omega_0$ and T/T_{D} only the term $n = 0$ is needed.

Then substitution of (I-10.2), the low-temperature and weak-coupling solution

$$(7.14) \quad \alpha \simeq \left(\frac{4\lambda\omega_0}{\pi\gamma^2} \cdot \frac{T}{T_{\text{D}}} \right)^2,$$

and according to (7.10) of

$$(7.14') \quad \frac{v_{\text{II}}}{v} - 1 \sim \frac{\alpha}{2}$$

yields the line shift to lowest order in all variables including the most important logarithmic terms

$$(7.15) \quad \Delta_q(-v_{\text{II}}|q|) \simeq v_{\text{II}}|q| \cdot 3 \left(\frac{\lambda\omega_0}{\pi\gamma^2} \cdot \frac{T}{T_D} \right) \cdot \left\{ -\frac{v_{\text{II}}|q|}{\gamma\omega_0} + 4 \left(\frac{\lambda\omega_0}{\pi\gamma^2} \cdot \frac{T}{T_D} \right) \cdot \frac{\lambda\omega_0}{\pi\gamma} \cdot \left[4 + 4 \left| \frac{v_{\text{II}}}{v_{\text{I}}} \cdot \frac{aq}{2} \right| \cdot \frac{1}{\gamma} \cdot \frac{T}{T_D} \log \left(\frac{\lambda\omega_0}{\pi\gamma^2} \cdot \frac{T}{T_D} \right) + \left| \frac{v_{\text{II}}}{v_{\text{I}}} \cdot \frac{aq}{2} \right|^2 \log \left(\left| \frac{v_{\text{II}}}{v_{\text{I}}} \cdot \frac{aq}{2} \right| \right) \right] \right\}.$$

The line width follows from (6.6) with (6.7) and (6.8) and is much easier to calculate, because the imaginary part of (6.7) for $z = -\Omega_q + i\varepsilon$ introduces δ -functions:

$$(7.16) \quad \Gamma_q(-\Omega_q) = \left(\frac{dF_q(z)}{dz} \Big|_{z=-\Omega_q} \right)^{-1} \cdot \frac{\pi\lambda}{\gamma^2} \otimes \frac{1}{N} \sum_k \{ \bar{\omega}_{k-q/2} \bar{\omega}_{k+q/2} \cdot (1 + \bar{n}_{k-q/2} + \bar{n}_{k+q/2}) \otimes \otimes \{ \delta(\bar{\omega}_{k-q/2} + \bar{\omega}_{k+q/2} + \Omega_q) - \delta(\bar{\omega}_{k-q/2} + \bar{\omega}_{k+q/2} - \Omega_q) \} \}.$$

The argument of the first δ -function vanishes only when $k = q = 0$, and then the whole factor vanishes so that only the second δ -function contributes. But if we take for the zero of $\bar{\omega}_{k-q/2} + \bar{\omega}_{k+q/2} - \Omega_q$ the linearized solution (7.6'), we find immediately a vanishing line width. This means that $\Gamma_q(-v_{\text{II}}|q|)$ is at least of order q^2 which follows indeed by setting instead of (7.6'), according to (7.2) and (7.5')

$$(7.17) \quad \sin \frac{ak_0}{2} = \frac{v_{\text{II}}|q|}{2\bar{\omega}_0 \cdot \cos aq/4}.$$

With $N^{-1} \sum_k$ taken as $(a/2\pi) \int dk$ for $N \rightarrow \infty$ and the substitution $\sin(ak/2) = x$ we find, choosing the integration limits such as to contain (7.17) and simultaneously to avoid change in sign of $\sin(a/2)(k \pm |q/2|)$:

$$\begin{aligned} \Gamma_q(-v_{\text{II}}|q|) &= \left(\frac{dF_q(z)}{dz} \Big|_{z=-v_{\text{II}}|q|} \right)^{-1} \cdot \frac{\lambda\omega_0}{\pi\gamma \cos aq/4} \otimes \\ &\otimes \int_{\sin|aq/2|}^1 \frac{dx}{\sqrt{1-x^2}} \cdot \delta \left(x - \frac{v_{\text{II}}|q|}{2\gamma\omega_0 \cos aq/4} \right) \cdot \left(x^2 - \sin^2 \frac{aq}{4} \right) \cdot \\ &\cdot \left(1 + \left(\exp \left[\beta\gamma\omega_0 \left(x \cdot \cos \frac{aq}{4} - \sqrt{1-x^2} \cdot \sin \frac{aq}{4} \right) \right] - 1 \right)^{-1} + \right. \\ &\quad \left. + \left(\exp \left[\beta\gamma\omega_0 \left(x \cdot \cos \frac{aq}{4} + \sqrt{1-x^2} \cdot \sin \frac{aq}{4} \right) \right] - 1 \right)^{-1} \right). \end{aligned}$$

Substitution of (I.8.3) for $dF_q(z)/dz|_{z=-v_{\text{II}}|q|}$ in the same approximation as for $\Delta_q(-v_{\text{II}}|q|)$, of (7.14) and of (7.4) gives to lowest order

$$(7.18) \quad \Gamma_q(-v_{\text{II}}|q|) \simeq -4! \frac{v_{\text{II}}^2 q^2}{\gamma\omega_0} \cdot \left(\frac{\lambda\omega_0}{\pi\gamma^2} \cdot \frac{T}{T_D} \right)^3.$$

8. – Conclusion.

The aim of this Part II is to justify *a posteriori* the approximation of phonon number conservation used in Part I. There we have proved for a monatomic linear chain the existence of a collective mode characterized by the creation operator (I-4.1)

$$(8.1) \quad c_a^* = \sum_k \alpha_{k,k-a}^* n_k(q),$$

where $n_k(q)$ is defined by (1.11).

The spectrum of the long-wavelength mode ($v_I|q| \ll (T/T_D)\omega_0$) according to (7.8) is soundlike and given by

$$(8.2) \quad \Omega_a \simeq v_{II}|q| + O\{|q|^2\}$$

in the approximation of I, the velocity v_{II} being related to the sound velocity v_I by (7.14'). For temperatures $T \ll T_D$ and weak coupling ($\lambda\omega_0 \ll 1$), the phonon renormalization γ within (7.14) can be neglected as may be seen from (I-9.2') and the collective energy is

$$(8.3) \quad v_{II}|q| \simeq v_I|q| + v_I|q| \cdot 8 \left(\frac{\lambda\omega_0}{\pi} \cdot \frac{T}{T_D} \right)^2.$$

In the phonon-number-nonconserving system considered here this energy is shifted by an amount of order

$$(8.4) \quad |\Delta_a(-v_{II}|q|)| \simeq v_{II}|q| \cdot 3 \left(\frac{\lambda\omega_0}{\pi} \cdot \frac{T}{T_D} \right) \cdot \left| \frac{16\lambda\omega_0}{\pi} \left(\frac{\lambda\omega_0}{\pi} \cdot \frac{T}{T_D} \right) - \frac{v_I|q|}{\omega_0} \right|,$$

which follows from taking the dominant terms of (7.15). The long-wavelength limit defined by $v_I|q|/\omega_0 \ll T/T_D$ can in particular be taken such that

$$(8.5) \quad \frac{v_I|q|}{\omega_0} \sim (\lambda\omega_0)^2 \cdot \frac{T}{T_D}$$

for weak coupling. Then (8.4) implies that the energy shift $|\Delta_a(-v_{II}|q|)|$ is one order smaller in the interaction $\lambda\omega_0$ than the difference between the collective energy (8.3) and the phonon energy $v_I|q|$. Thus the phonon-number-conserving approximation of Part I gives the correct collective velocity v_{II} in lowest order of $\lambda\omega_0$. The phonon-number-nonconserving interactions not only renormalize v_{II} through a factor $\sim \lambda\omega_0$ but they are also responsible for the deviation of the collective-mode spectrum $\Omega(q)$ from the straight line (8.3). In addition

the line width $|I_a(-v_{\text{II}}|q)|$ given by (7.18) is smaller than the line shift (8.4) by a factor

$$\sim \frac{T}{T_D} \cdot \frac{v_{\text{I}}|q|}{\omega_0} \ll \left(\frac{T}{T_D}\right)^2 \ll 1,$$

assuming (8.5). In other words, the collective mode which is due essentially to the phonon-number-conserving interactions is not destroyed by the phonon-number-nonconserving ones.

So far, the linear chain is of little physical interest, except perhaps some modified application to organic molecular chains. But the proof for the existence of a collective mode in a one-dimensional system of phonons enables one to clarify the problem of the existence of such a mode in three-dimensional crystals.

The problem for the formalism to be used to possibly establish the existence of a collective mode consists in finding linear relations between two-phonon operators or, equivalently, between two-phonon Green functions. We succeeded in doing so by the equation of motion method or by the generalized Bethe-Salpeter equations, but in both methods, a solution has only been found under certain conditions.

These conditions formulated quite generally in the Introduction of Part I remain the same for three-dimensional crystals. But the factorization property of the anharmonic coefficients after unitary transformation of the Hamiltonian cannot be obtained exactly, even in the limit of small momentum. Now the properties specific for the linear chain which guarantee the factorization in this work are of three types. There is first the fact that the anharmonic coefficients for the chain are (Part I, Appendix B.2)

$$(8.6) \quad C_{k_1, \dots, k_n}^{(n)} = \text{const } (\omega_{k_1} \dots \omega_{k_n})^{\frac{1}{2}} \mathcal{A}\left(\sum_i k_i\right).$$

This form follows from that of the unique phonon branch

$$(8.7) \quad \omega_k = \omega_0 \cdot \sin\left(\frac{ak}{2}\right),$$

which is the most important point for the factorization, because the addition formula for the trigonometric functions can be used in the calculation of the anharmonic coefficients in $:\hat{H}:$ (see Appendix D).

Three-dimensional perfect crystals not only have more than one branch, but no analogue to (8.6) is known to hold exactly. In ref. (4) eq. (8.6) is postulated and the validity of such a model discussed. We presume that for this

(4) I. P. IPATOWA, A. A. MARADUDIN and R. F. WALLIS: *Phys. Rev.*, **155**, 882 (1967).

model a collective mode may be found, provided that a suitable form for the phonon frequencies can be used which guarantees the factorization of the coefficients (5.11) and also has the symmetry of the specific crystal considered. Indeed, a very crude calculation with two simple and unrealistic models, the one isotropic, the other highly anisotropic, established that changing the symmetry changes radically the result. Consequently the first step towards establishing a three-dimensional collective mode of phonons consists in characterizing their spectrum by trigonometric functions which have the right symmetry, and which are in agreement with measured phonon dispersion curves.

* * *

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APPENDIX D

Coefficients of $:\tilde{H}:$ for special indices.

In addition to the long-wavelength limit ($|q| \ll \pi/a$) of $\tau_{(q-k, -k')(k, k'-q)}$ calculated in Appendix C (part I) we need in the same limit $\tau_{(-k-q, k)(k'+q, -k')}$, $\nu_{-k-q, (-k', k, k'+q)}$ and $\mu_{(k, -k-q, -k', k'+q)}$ defined in Appendix A (part I). In Appendix C we have shown that for any algebraic function f

$$\begin{aligned} \sum_i C_{k_1, k_2, i}^{(3)} C_{\tilde{k}_3, k_4, -i}^{(3)} f(\omega_i; \omega_{k_1}, \omega_{k_2}, \omega_{k_3}, \omega_{k_4}) = \\ = N^{-1} \lambda_2^2 \lambda_2^{-3} \cdot (\omega_{k_1} \cdot \omega_{k_2} \cdot \omega_{k_3} \cdot \omega_{k_4})^{\frac{1}{2}} \cdot \tilde{A} \left(\sum_{i=1}^4 k_i \right) \cdot \omega_{k_1+k_2} \cdot f(\omega_{k_1+k_2}; \omega_{k_1}, \omega_{k_3}, \omega_{k_4}, \omega_{k_4}). \end{aligned}$$

Applying this rule to the quantities defined in Appendix A we get

$$(D.1) \quad B_{(-k-q, k)(k'+q, -k')}^{(2)} = -3! \lambda_3^2 \lambda_2^{-3} N^{-1} \cdot (\omega_{k+q} \omega_k \omega_{k'+q} \omega_{k'})^{\frac{1}{2}} \cdot \beta'_{k, k'}(q),$$

$$(D.2) \quad B_{-k-q, (-k', k, k'+q)}^{(3)} = -4 \lambda_3^2 \lambda_2^{-3} N^{-1} \cdot (\omega_{k+q} \omega_k \omega_{k'+q} \omega_{k'})^{\frac{1}{2}} \cdot \gamma_{k, k'}(q),$$

$$(D.3) \quad B_{(k, -k-q, -k', k'+q)}^{(4)} = - \lambda_3^2 \lambda_2^{-3} N^{-1} \cdot (\omega_{k+q} \omega_k \omega_{k'+q} \omega_{k'})^{\frac{1}{2}} \cdot \delta_{k, k'}(q),$$

where

$$(D.1') \quad 2\beta'_{k,k'}(q) = \frac{\omega_q^2}{\omega_q^2 - (\omega_{k+q} + \omega_k - i\varepsilon)^2} + \frac{\omega_q^2}{\omega_q^2 - (\omega_{k'+q} + \omega_{k'} + i\varepsilon)^2} +$$

$$+ \frac{\omega_{k'-k}^2}{\omega_{k'-k}^2 - (\omega_{k'+q} - \omega_{k+q} + i\varepsilon)^2} + \frac{\omega_{k'-k}^2}{\omega_{k'-k}^2 - (\omega_{k'} - \omega_k + i\varepsilon)^2} +$$

$$+ \frac{\omega_{k+k'+q}^2}{\omega_{k+k'+q}^2 - (\omega_{k'} - \omega_{k+q} + i\varepsilon)^2} + \frac{\omega_{k+k'+q}^2}{\omega_{k+k'+q}^2 - (\omega_{k'+q} - \omega_k + i\varepsilon)^2},$$

$$(D.2') \quad 2\gamma_{k,k'}(q) = \frac{\omega_{k-k'}^2}{\omega_{k-k'}^2 - (\omega_{k'+q} - \omega_{k+q} + i\varepsilon)^2} + \frac{\omega_{k-k'}^2}{\omega_{k-k'}^2 - (\omega_{k'} + \omega_k + i\varepsilon)^2} +$$

$$+ \frac{\omega_{k+k'+q}^2}{\omega_{k+k'+q}^2 - (\omega_{k'} - \omega_{k+q} + i\varepsilon)^2} + \frac{\omega_{k+k'+q}^2}{\omega_{k+k'+q}^2 - (\omega_{k'+q} + \omega_k + i\varepsilon)^2} +$$

$$+ \frac{\omega_q^2}{\omega_q^2 - (\omega_k - \omega_{k+q} + i\varepsilon)^2} + \frac{\omega_q^2}{\omega_q^2 - (\omega_{k'} + \omega_{k'+q} + i\varepsilon)^2},$$

$$(D.3') \quad 2\delta_{k,k'}(q) = \frac{\omega_{k+k'+q}^2}{\omega_{k+k'+q}^2 - (\omega_{k+q} + \omega_{k'} + i\varepsilon)^2} + \frac{\omega_{k+k'+q}^2}{\omega_{k+k'+q}^2 - (\omega_k + \omega_{k'+q} + i\varepsilon)^2} +$$

$$+ \frac{\omega_{k-k'}^2}{\omega_{k-k'}^2 - (\omega_{k+q} + \omega_{k'+q} + i\varepsilon)^2} + \frac{\omega_{k-k'}^2}{\omega_{k-k'}^2 - (\omega_k + \omega_{k'} + i\varepsilon)^2} +$$

$$+ \frac{\omega_q^2}{\omega_q^2 - (\omega_{k'} + \omega_{k'+q} + i\varepsilon)^2} + \frac{\omega_q^2}{\omega_q^2 - (\omega_k + \omega_{k+q} + i\varepsilon)^2}.$$

Substitution of (D.1), (D.2) and (D.3) into the definitions of Appendix A gives with (B.2) of Appendix B (Part I):

$$(D.4) \quad 4\tau_{(-k-q,k)(k'+q,-k')} = 3! N^{-1} \lambda_2^{-3} \cdot (\lambda_4 \lambda_2 - \lambda_3^2 \beta'_{kk'}(q)) \cdot (\omega_k \omega_{k+q} \omega_{k'} \omega_{k'+q})^{\frac{1}{2}},$$

$$(D.5) \quad \nu_{-k-q,(-k',k,k'+q)} = N^{-1} \lambda_2^{-3} \cdot (\lambda_4 \lambda_2 - \lambda_3^2 \gamma_{k,k'}(q)) \cdot (\omega_k \omega_{k+q} \omega_{k'} \omega_{k'+q})^{\frac{1}{2}},$$

$$(D.6) \quad 4\mu_{(k,-k-q,-k,k'+q)} = N^{-1} \lambda_2^{-3} \cdot (\lambda_4 \lambda_2 - \lambda_3^2 \delta_{k,k'}(q)) \cdot (\omega_k \omega_{k+q} \omega_{k'} \omega_{k'+q})^{\frac{1}{2}}.$$

Now $\lambda_4 \lambda_2$ and λ_3^2 are of the same order of magnitude, which enables us to take to lowest order in $|q|$, the limit $|q| \rightarrow 0$ for the functions β' , γ and δ . The result is

$$(D.4') \quad \beta'_{k,k'}(0) = 1 + \mathbf{P} \frac{\omega_0^2}{\omega_k \omega_{k'}},$$

$$(D.5') \quad \gamma_{k,k'}(0) = 1,$$

$$(D.6') \quad \delta_{k,k'}(0) = 1 - \mathbf{P} \frac{\omega_0^2}{(\omega_k \omega_{k'})},$$

where $\mathbf{P}$ denotes the principal value.

Let us see in some detail how *e.g.* (D.4') is obtained. We insert

$$\frac{1}{x \pm i\varepsilon} = \mathbf{P} \frac{1}{x} \mp i\pi\delta(x)$$

and the phonon spectrum (B.1) in (D.1').

Because in (D.4) $\beta'_{k,k'}(q)$ multiplies $(\omega_k \omega_{k+q} \omega_{k'} \omega_{k'+q})^{\frac{1}{2}}$ and this product appears only in integrals where the other factor of the integrand is regular for $\omega_k = 0$ and $\omega_{k+q} = 0$, none of the δ -functions will give a nonzero contribution. We have therefore

$$\beta_{k,k'}(0) = \mathbf{P} \left\{ \frac{\omega_{k'-k}^2}{\omega_{k'-k}^2 - (\omega_{k'} - \omega_k)^2} + \frac{\omega_{k'+k}^2}{\omega_{k'+k}^2 - (\omega_{k'} - \omega_k)^2} \right\},$$

$$\omega_{k' \pm k}^2 = \omega_0^2 \left(\sin^2 \frac{ak'}{2} + \sin^2 \frac{ak}{2} \pm 2 \sin \frac{ak'}{2} \sin \frac{ak}{2} \cos \frac{a(k' \pm k)}{2} \right),$$

and with

$$\left| \sin \frac{ak}{2} \right| \equiv \sigma(k) \sin \frac{ak}{2},$$

$$\beta'_{k,k'}(0) = \frac{\mathbf{P}}{2|\sin ak/2| \cdot |\sin ak'/2|} \cdot \frac{N(k, k')}{D(k, k')},$$

where

$$N(k, k') = \left(\sin^2 \frac{ak}{2} + \sin^2 \frac{ak'}{2} \right) \cdot \left(2 - \sigma(k)\sigma(k') \left[\cos \frac{a(k-k')}{2} - \cos \frac{a(k+k')}{2} \right] \right) -$$

$$- 2 \sin \frac{ak}{2} \sin \frac{ak'}{2} \left(\cos \frac{a(k-k')}{2} - \cos \frac{a(k+k')}{2} + \right.$$

$$\left. + 2\sigma(k)\sigma(k') \cos \frac{a(k+k')}{2} \cdot \cos \frac{a(k-k')}{2} \right),$$

$$D(k, k') = 1 - \sigma(k)\sigma(k') \left(\cos \frac{a(k-k')}{2} - \cos \frac{a(k+k')}{2} \right) - \cos \frac{a(k-k')}{2} \cdot \cos \frac{a(k+k')}{2};$$

with

$$\cos \frac{a(k-k')}{2} - \cos \frac{a(k+k')}{2} = 2 \sin \frac{ak}{2} \cdot \sin \frac{ak'}{2}$$

and

$$2 \cos \frac{a(k-k')}{2} \cdot \cos \frac{a(k+k')}{2} = \cos ak + \cos ak'$$

follows

$$\begin{aligned}
 N(k, k') - 2 \left| \sin \frac{ak}{2} \right| \cdot \left| \sin \frac{ak'}{2} \right| \cdot D(k, k') = \\
 = 2 \left(\sin^2 \frac{ak}{2} + \sin^2 \frac{ak'}{2} \right) \cdot \left(1 - \left| \sin \frac{ak}{2} \right| \cdot \left| \sin \frac{ak'}{2} \right| \right) - \\
 - \left| \sin \frac{ak}{2} \right| \cdot \left| \sin \frac{ak'}{2} \right| \cdot (2 + \cos ak + \cos ak') .
 \end{aligned}$$

Writing

$$2 \left(\sin^2 \frac{ak}{2} + \sin^2 \frac{ak'}{2} \right) = 2 - (\cos ak + \cos ak') ,$$

one finds

$$N(k, k') - 2 \left| \sin \frac{ak}{2} \right| \cdot \left| \sin \frac{ak'}{2} \right| \cdot D(k, k') = 2D(k, k') ,$$

which leads to (D.4'). The same procedure is used for finding (D.5') and (D.6')
 With $4\lambda \equiv (\lambda_4 \lambda_2 - \lambda_3^2) \cdot \lambda_2^{-3}$ the result is

$$(D.7) \quad \tau_{(-k-q, k), (k'+q, -k')} \simeq 3! N^{-1} \lambda \cdot (\omega_k \omega_{k+q} \omega_{k'} \omega_{k'+q})^{\frac{1}{2}} - \frac{(\omega_0 \lambda_3)^2}{4N \lambda_2^3} \mathbf{P} \left(\frac{\omega_{k+q} \omega_{k'+q}}{\omega_k \omega_{k'}} \right)^{\frac{1}{2}} ,$$

$$(D.8) \quad \nu_{-k-q, (-k', k, k'+q)} \simeq 4 N^{-1} \lambda \cdot (\omega_k \omega_{k+q} \omega_{k'} \omega_{k'+q})^{\frac{1}{2}} ,$$

$$(D.9) \quad \mu_{(k, -k-q, -k', k'+q)} \simeq N^{-1} \lambda \cdot (\omega_k \omega_{k+q} \omega_{k'} \omega_{k'+q})^{\frac{1}{2}} + \frac{(\omega_0 \lambda_3)^2}{4N \lambda_2^3} \mathbf{P} \left(\frac{\omega_{k+q} \omega_{k'+q}}{\omega_k \omega_{k'}} \right)^{\frac{1}{2}} .$$

